T. Dickie

# ONTARIO'S WATER QUALITY OBJECTIVE DEVELOPMENT PROCESS

MAY 1991

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1991

Ontario

Environment
Environnement

ISBN 0-7729-7532-9

# ONTARIO'S WATER QUALITY OBJECTIVE DEVELOPMENT PROCESS

AQUATIC CRITERIA DEVELOPMENT COMMITTEE
WATER RESOURCES BRANCH
ONTARIO MINISTRY OF THE ENVIRONMENT

MAY 1991

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## ABSTRACT

As part of its program to ensure that the surface waters of Ontario are satisfactory for aquatic life and recreation, the Ontario Ministry of the Environment develops Provincial Water Quality Objectives (PWQOs) and Guidelines (PWQGs). This report details the procedures used to develop PWQOs and PWQGs. PWQOs are developed from the best available knowledge on the effects of substances on aquatic life. Data are required for acute and chronic toxicity, bioaccumulation and mutagenicity. Also considered is available information on environmental fate, physical-chemical properties, taste and odour in water and tainting of fish tissues. If adequate information is unavailable for setting a PWQO, a PWQG is developed using uncertainty factors which depend on the quantity and quality of the toxicological data.

## RESUME

En formant parti de la programme pour assurer que la qualité des eaux de surface de la province de l'Ontario suffise pour supporter la vie aquatique et la récréation, le Ministère de l'Environnement de l'Ontario dévelope des Objectifs Provinciaux pour la Qualité des Eaux (OPQE) et des Normes Provinciaux pour la Qualité des Eaux (NPQE). Ce rapport donne les détails nécessaires pour développer les OPQEs et les NPQEs. Les Objectifs Provinciaux pour la Qualité des Eaux sont établi par une connaissance le meilleur possible des effets des agents chimiques sur la vie aquatique. Des informations sont requises concernant la toxicité aigue et chronique, la bioaccumulation, et la mutagénicité. Autres renseignements considérés sont le sort dans l'environnement, les propriétés physico-chimique, goût et odeur dans l'eau, et le potentiel pour corrompre la chair des poissons. Jusqu'à temps que l'information ne suffise pour développer un OPQE, une NPQE est determinée. Pour développer une Norme, on applique plusieurs facteurs d'incertitude qui dépendent sur la qualité et la quantité de l'information toxicologique.

## ACKNOWLEDGEMENTS

This document is the product of the Aquatic Criteria Development Committee. What started out as an attempt to formalize existing procedures for developing PWQOs turned into a reassessment of the process itself. The following people made significant contributions to the document through discussions within the committee and in writing drafts:

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The tables and figures were prepared by Tom Dickie, Tim Fletcher and Natalie Waddell.

The final draft report was widely circulated across Canada and the United States for scientific peer review. Many comments and suggestions were received, all were carefully evaluated and appropriate changes were subsequently made to the document. The Aquatic Criteria Development Committee appreciates the assistance of all those people who contributed their time and knowledge to the completion of this document.

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# 1 INTRODUCTION

## 1.1 The Basis for Provincial Water Quality Objectives

The mandate for water quality management in Ontario is legislated under several statutes, most notably, the Water Resources Act. In addition, the Ministry of the Environment has specific policies (MOE, 1984) with the goal:

> *"to ensure that the surface waters of the province are of a quality which is satisfactory for aquatic life and recreation."*

To support this goal, the Ministry's policy further states that:

> *"... the Objectives are set at such values as to protect all forms of aquatic life and all aspects of the aquatic life cycles. The clear intention is to protect all life stages during indefinite exposure to the water."*

In order to achieve these water management goals, a comprehensive understanding of, and sound management program for the control of physical, chemical and bacteriological pollutants is required. Since 1978, Ontario has relied on Provincial Water Quality Objectives and Guidelines as principal tools for surface water quality management.

Objectives are numerical and narrative values designed to protect all stages of aquatic life cycles during indefinite exposure to the water. The purpose of this document is to set forth detailed procedures for developing Provincial Water Quality Objectives (PWQOs). The PWQO development process closely adheres to the water management policy of the Ministry by requiring that PWQO setting considers a wide variety of representative aquatic organisms, critical life stages and toxic effects, including mutagenicity. To expand the assessment beyond direct toxic effects, the PWQO development process also considers bioaccumulation and taste and odour in water and tainting of fish tissues. The following factors are employed:

**Mandatory factors:**

- Toxicity to aquatic life (acute, chronic, lethal, sublethal)
- Bioaccumulation (Animals consuming aquatic organisms and humans consuming sport fish)
- Mutagenicity to aquatic life

**Other factors:**

- Fate and physical-chemical factors
- Sources and ambient levels
- Taste and odour in water and tainting of fish tissues
- Impacts on wildlife
- Recreation
- Sediment quality
- Objectives of other agencies (for comparison only).

PWQO setting is not influenced by analytical limitations, economics, social factors, or waste treatment availability. All of these are important in water management, and are considered in the site-specific

application of the Objectives. PWQOs are designed to take into account both cold-water and warm-water environments in a single Objective, with the exception of dissolved oxygen. An assessment of toxicity to both cold and warm-water species is a requirement of the PWQO setting process. Consequently, Objectives will be applied independent of the nature of the possible resident species (e.g. cold-water or warm-water species), the type of waterbody (lake or stream) and its trophic status.

The influence of water temperature and other specific physical and chemical factors such as pH and hardness are, however, considered when they affect the toxicity of the candidate substances for PWQO setting. The PWQO for ammonia, for example, is related to both pH and water temperature and the Objectives for many of the metals are related to water hardness.

The process of developing PWQOs has evolved with experience so that it is effective at taking into account crucial aspects of the hazard of substances in aquatic environments. The process is also efficient at developing Objectives and Guidelines with limited resources. The purpose of this document is to describe this process. By doing so, the applicability as well as the limitations of the Objectives will better be understood by water quality managers, by the public, as well as by those who assist in the process.

## 1.2 The Basis for Provincial Water Quality Guidelines

It is recognized that, for many substances of concern, there are not sufficient toxicological or other data to prepare a PWQO. In an effort to achieve a consistent approach in establishing environmental protection values for substances with limited information, a process for setting Provincial Water Quality Guidelines (PWQG) was established.

The PWQG setting process was developed to parallel, as closely as possible, the Objective setting process by employing toxicological data as well as considering bioaccumulation, mutagenicity and other factors, yet permitting the development of substance-specific environmental protection values with even a small amount of data. The PWQG process sets a margin of uncertainty whose size is dependent on the quantity and quality of available data. The process encourages the publication of new aquatic toxicity data to further refine the PWQG or allow it to become a PWQO.

## 1.3 Application of PWQOs and PWQGs

This document is not intended to describe in detail the application of Objectives and Guidelines in Ontario's water quality management programs. Objectives and Guidelines are designed for application to all surface waters (rivers, streams, lakes, etc.) in Ontario regardless of their existing use or condition. With specific respect to the use of PWQOs and PWQGs, the Ministry's surface water quality management goal is supported by a series of policies and application procedures. Key policies state:

> *"In areas which have water quality better than the Provincial Water Quality Objective* [or Guideline], *water quality shall be maintained at or above the Objectives* [or Guidelines]",

and

*"Water quality which presently does not meet the Provincial Water Quality Objectives* [or Guidelines] *shall not be degraded further and all practical measures shall be taken to upgrade the water quality to the Objectives* [or Guidelines]."

PWQOs and PWQGs are, therefore, used in combination with water quality monitoring data to assess ambient conditions in Ontario and to identify areas with existing or potential water quality problems.

The PWQO development process follows the policy of the Ministry to treat all surface waters in the province alike, except for distinguishing between waters that are of acceptable quality and those that are degraded. It is essential therefore to set Objectives that are stringent enough to protect the most sensitive environments.

Although Objectives and Guidelines are not legal standards *per se*, they are employed in various types of water quality models to establish acceptable wastewater loading limits on a site-specific basis. These loading limits, contained in Control Orders or other similar instruments, are legally enforceable.

The Ministry's water management policy lists several substances with "zero tolerance limits" which "... should be completely eliminated [from discharges]". The Municipal and Industrial Strategy for Abatement (MISA) is based on the goal of the virtual elimination of persistent toxic substances from point source discharges. Both of these policies relate to effluent control and in regulatory instruments they may supersede waste loading limits derived from a PWQO or PWQG. Objectives and Guidelines are needed, to assess the aquatic environmental significance of the materials that may be found in waterbodies as the result of spills and uncontrolled sources, and to protect local water quality in situations where technology based requirements may not be stringent enough to protect aquatic life.

PWQOs are set for individual chemicals or homologous groups and, for the most part, do not account for joint toxicity (i.e. additive, synergistic or antagonistic effects) resulting when a mixture of hazardous substances is present in a waterbody. In application, models addressing combined toxic effects should be employed wherever possible. At the very least, water quality managers should consider that waters with a quality at or near the Objectives for several parameters may not afford adequate protection to aquatic life. The empirical approach of testing whole effluent or receiving water samples directly addresses the joint toxicity of complex mixtures of substances.

## 1.4 Other Water Quality Objectives and Guidelines

PWQO's and PWQG's are designed primarily to meet the Ministry's goal of protecting aquatic life and recreational uses. There are other uses and criteria that should be considered. The Canadian Water Quality Guidelines (CCREM, 1987) for agricultural uses (irrigation and livestock watering) and industrial water supply provide protection for these uses and should be considered where applicable.

PWQOs are not Drinking Water Objectives and thus do not apply to drinking water. The Ministry has set Drinking Water Objectives which apply specifically to finished drinking water and not raw water. These Objectives are developed

independently of the PWQOs and are listed with supporting documentation in the MOE publication "Ontario Drinking Water Objectives" (MOE, 1983).

## 1.5 Water Quality Objective Setting Administrative Structure

The setting of PWQOs is primarily the responsibility of the Water Resources Branch of the Ontario Ministry of the Environment. Currently, the Aquatic Criteria Development Committee is responsible for all activities related to the development of Provincial Water Quality Objectives and Guidelines. This committee is comprised of staff of the Water Resources Branch, Hazardous Contaminants Coordination Branch, Laboratory Services Branch, Investigations and Enforcement Branch, the MOE Regions and Environment Canada.

## 1.6 What are Objectives and Guidelines? – A Definition of Terms

Throughout this report, references are made to *Objectives* and *Guidelines*. There are many government agencies using these terms throughout the world and they each have their own definitions. For water quality management in Ontario, the terms are defined as:

### 1.6.1 Objective

A Provincial Water Quality Objective (PWQO) is a numerical or narrative limit recommended to protect all forms of aquatic life and all aspects of the aquatic life cycles during indefinite exposure and to protect recreational water uses. Objectives are established when a defined minimum information base is available. They are used to assess ambient surface water quality, identify areas with degraded conditions, assess impacts of wastewater discharges and spills, and provide a basis for establishing industrial and municipal wastewater discharge limits.

### 1.6.2 Guideline

For many substances there are some scientifically sound aquatic toxicological data available with which to assess potential aquatic environmental impacts, but there is not enough information to meet the minimum requirements for setting a PWQO. In these cases, the available data are assessed and, using a prescribed method of applying uncertainty factors determined by the quality and quantity of data, a Guideline value is calculated. This PWQG represents the best available value and is employed the same way as a PWQO with the understanding that it is more likely to change as additional information becomes available. Guidelines are recommended with the intention of upgrading them to PWQO status as sufficient information becomes available.

### 1.6.3 Interim Guideline

An Interim Guideline is a numerical water quality limit set using the Provincial Water Quality Guideline procedures, normally, to meet an emergency need for the Ministry of the Environment. It is based on a search of the best information at hand. An Interim Guideline is set by qualified Ministry staff and then checked and approved by other senior Ministry scientists. Unlike the PWQO or PWQG, an Interim Guideline is not subject to a formal peer review or further Ministry approval and publication.

## 1.7 Priority of Candidate Substances for PWQOs

The availability of toxicological data is limited for many of the substances now being detected. With the rapidly expanding capabilities of analytical chemists to measure contaminants in the environment, those responsible for the setting of water quality Objectives face a major challenge to keep pace. In addition, there is an increasing need to develop PWQOs for the constituents of complex effluents.

In order to make the most efficient use of resources and scientific data, most agencies develop priority substance lists. Ontario has lists in the areas of air, waste and water resources management. Resource limitations may also preclude the possibility of setting environmental protection values for all substances in the short term. Consequently, the absence of a published PWQO or PWQG for a substance does not necessarily mean that it is harmless or that action will not be taken eventually.

The development of a water quality Objective takes a wide variety of effects into consideration. In order to achieve consistency in the process and to efficiently employ available resources, a comprehensive and systematic approach has been developed.

The Ministry developed a screening process to identify a list of contaminants of greatest concern for Ontario. This list, the Effluent Monitoring Priority Pollutants List (EMPPL), is supported by a published document (MOE, 1987). The screening process consisted of a chemical identification stage and a preliminary hazard assessment stage. A number of factors were considered for each chemical. These include: potential presence in effluent, persistence, potential to bioaccumulate, and acute and chronic toxicity to organisms, including humans. The substances on the list have been derived from an ongoing assessment process which so far has considered in excess of 1500 chemicals. Substances currently not on the EMPPL but identified through complete characterization of effluent samples will be candidates for inclusion on the EMPPL. Chemicals may also be added to reflect new information on environmental fate or toxicity.

This list is used to establish priorities for Objective setting. Data on environmental persistence, bioaccumulation, fate and aquatic toxicity data are assessed and the substances are categorized in terms of their potential impact on the aquatic communities and uses such as fish consumption. Objectives are being set for EMPPL substances with the highest potential for impairment and the intention is to establish Objectives or Guidelines for all of the EMPPL substances as rapidly as resources and the availability of data permit.

Requests for Objectives are received from MOE Regional and Branch staff. Such requests are ranked in order of priority and assessed as soon as possible.

## 1.8 Summary of PWQO and PWQG Setting

The following briefly describes the key components of the process and provides reference to detailed discussions in subsequent chapters of this document (Figure 1).

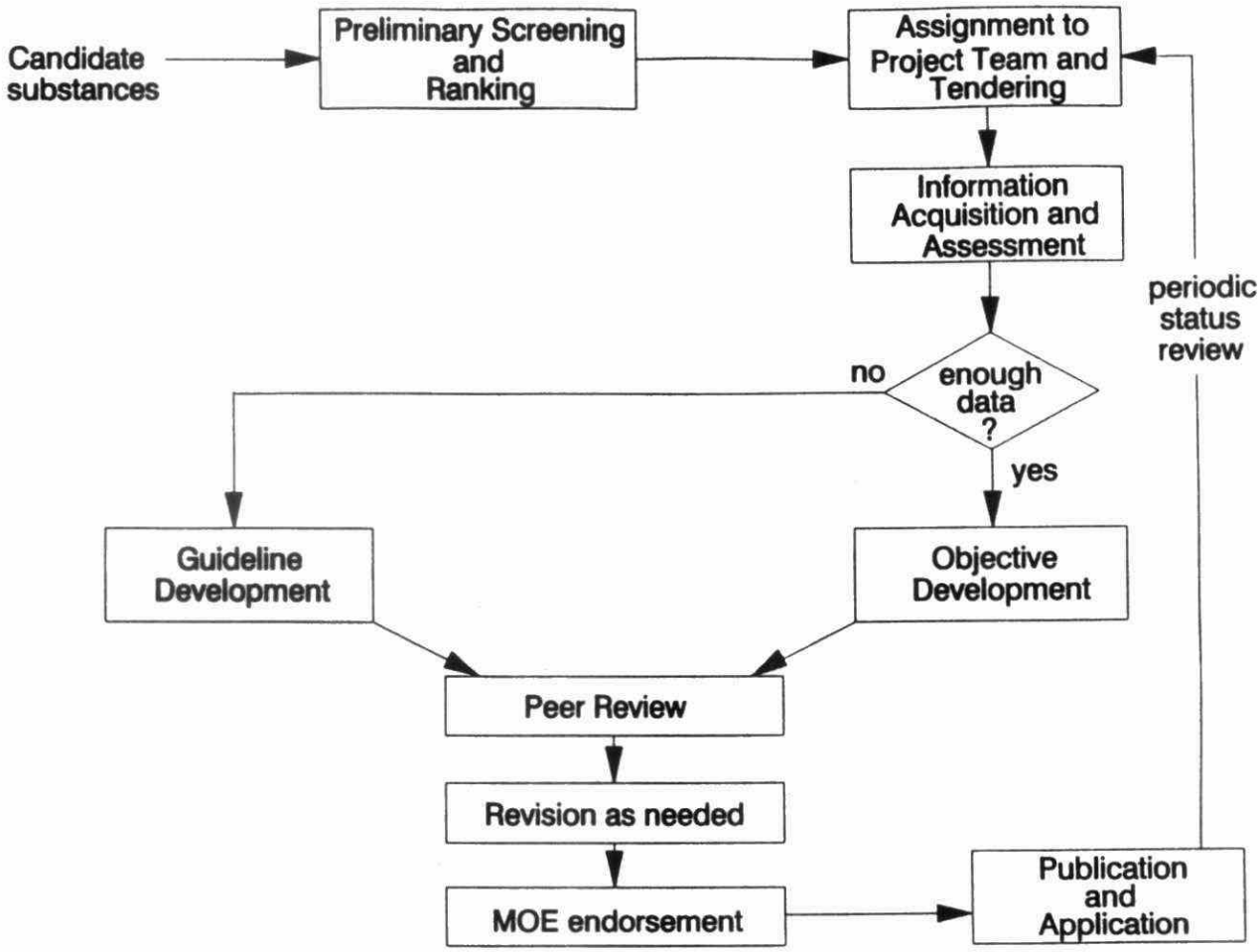


Figure 1. The process for developing PWQOs and PWQGs

### 1.8.1 Selection of Candidate Substances

Requests for new Objectives originate in various pollution control activities of the Ministry of the Environment and from other Ministries. Candidate substances are screened for existing or potential hazard and occurrence in the aquatic environment. They are then ranked for immediate or future action.

To satisfy the immediate need for an Objective, an Interim Guideline may be set. Based on the results of the Interim Guideline setting, Interim Guidelines may be recommended for PWQO or PWQG development.

### 1.8.2 Assignment

An Objective development document is prepared by a Ministry project team, normally with the assistance of a consultant.

### 1.8.3 Information Acquisition and Assessment

The world literature is searched for information that will be needed for setting a

PWQO. The reviewer is seeking information on aquatic toxicity, bioaccumulation, taste and odour in water or tainting of fish tissues, mutagenicity, fish consumption limits, impacts on wildlife, environmental fate, sources, objectives of other agencies, and, any other appropriate information found in the literature search.

The information so obtained is then assessed. Rules for the adequacy and admissibility of data on aquatic toxicity, bioaccumulation and tainting are described later in this document. All candidate information is screened for acceptability. Refereed publications are preferred. The fact that information is published is not sufficient, however, to justify its use in PWQO development.

### 1.8.4 Setting a Provincial Water Quality Objective

Provincial Water Quality Objectives are set to protect aquatic life and recreational water uses. The assessment of aquatic toxicity data is fundamental to the process but other factors such as bioaccumulation, taste and odour in water and tainting of fish tissues, mutagenicity, wildlife protection, and recreation and aesthetics are also considered. Further details are provided in Chapter 2 of this document. Information on the aquatic environmental fate is included for reference.

The final draft report of the Objective Development Document is reviewed by staff of the Ministry of the Environment and forwarded to recognized experts in Canada and other countries.

The comments of the reviewers are assessed and appropriate revisions or additions are made to the draft report. The final report is submitted for approval and publication by the Ministry.

### 1.8.5 Setting a Provincial Water Quality Guideline

Once all of the information is obtained and assessed, a decision is made as to whether a PWQO can be set. If sufficient toxicological information (which meets MOE rules for admissibility) is available then a PWQO can be set.

When some aquatic toxicological data are available, but the minimum data set requirements for a PWQO cannot be met, a PWQG can usually be calculated. As in the Objective setting process, the Guideline process begins by selecting a value based on the lowest toxic effect concentration for an appropriate aquatic species and dividing that value by an uncertainty factor. The magnitude of the uncertainty factor is determined by the quantity and quality of available toxicity data and the physical-chemical properties of the substance. The Guideline setting process has a screening mechanism to accommodate concerns about bioaccumulation. Like the PWQO setting process, the Guideline setting process also considers mutagenicity. A numeric Guideline based on mutagenicity will only be set for substances with demonstrated mutagenic properties and where data for aquatic organisms are available.

This Guideline process begins by selecting a value based on the lowest mutagenicity-related effect in the most sensitive aquatic species. This value is divided by an uncertainty factor, whose magnitude is based on the quantity and quality of mutagenicity data and physical-chemical properties of the substance.

The development of a Guideline can also consider factors such as taste and odour in water and fish tissue tainting. Further

details are provided in Chapter 3 of this document.

The final draft of the Guideline Development Document is reviewed by staff of the Ministry of the Environment and forwarded to recognized experts in Canada and other countries. The Guideline is then submitted for approval and publication by the Ministry.

# 2 SETTING PROVINCIAL WATER QUALITY OBJECTIVES

## 2.1 Substance Physical-Chemical Properties

The fate and effects of organic contaminants in aquatic systems are largely determined by their inherent physical-chemical properties. Hence a knowledge of the fundamental substance properties (e.g. octanol-water partition coefficient) is essential in any assessment of potential environmental effects. Where this information is available, it is included in the PWQO development document.

## 2.2 Acute and Chronic Toxicity

PWQOs are primarily developed using the available knowledge of aquatic toxicity of the substances to which they refer. Many people relate aquatic toxicity with the survival of fish but the development of PWQOs also considers other impacts on aquatic life. A substance is generally considered toxic if it reduces longevity, fecundity, growth, reproductive success, produces atypical behaviour, physiological effects, histological effects or deformities, including tumours. Ontario's Water Quality Objectives are intended to provide limits for substances in fresh water environments. If these limits are achieved, observable deleterious impacts are unlikely. Since the PWQOs are intended to protect Ontario's fresh water environments, data relating to fresh water aquatic life resident in the province must be included.

### 2.2.1 Acute Versus Chronic Tests

Since it makes little sense to protect aquatic life only from short term exposures to toxic substances, PWQOs are primarily based on the results of chronic test exposures. Decisions regarding exposure durations are complex and are assessed on a case by case basis.

An acute effect comes rapidly to an end--point while a chronic effect is long lasting or continued. The words acute and chronic in connection with toxicity tests refer to short (acute) and long (chronic) exposure. Such terms require a specific organism as a reference. For a *Daphnia* with a life cycle of weeks, acute usually means two days or less. Acute effects are not synonymous with lethal effects. However, for trout with a life cycle of years, acute usually means four days or less. Lethality caused by chronic exposure is a valid observation for PWQO development. In considering the appropriateness of the exposure duration, some consideration should be given to the nature of the toxicant itself.

Lethal or effective concentrations for some substances (e.g. zinc, phenol) are similar whether they relate to four day exposure or 30 day exposure, while other toxicants (e.g. methyl-mercury, DDT) accumulate for the entire life of the organism (see Appendix A for detailed discussion). For PWQO development, the results of shorter term tests are considered if it can be demonstrated that all the observed impacts are expected to occur within the exposure period.

Also important, are sublethal effects which occur at lower concentrations. Some judgement must be made as to whether these effects are harmful to the organism.

### 2.2.2 Primary and Secondary Data

All candidate toxicological information is screened for acceptability. All information that meets the following requirements is considered primary data:

- Toxicity tests must employ accepted laboratory practices of exposure and environmental controls. While all tests must be evaluated on a case by case basis, those tests following published protocols of government agencies or standard setting associations are generally acceptable.

- Any tests may be acceptable, including static tests if it can be shown that concentrations of the toxicant are not changing (significantly) throughout the test and adequate environmental conditions for the test species are maintained with respect to such factors as dissolved oxygen and accumulation of metabolic wastes. Generally, continuous flow exposures, and renewal tests (i.e. static tests with replacement) are acceptable if appropriate rates of renewal of toxicant are maintained. Static tests are acceptable if concentrations of the toxicant are measured in the exposure vessel at the beginning and end of the test and no more than 10% of the toxicant is lost during the test.

- Dissolved concentrations of toxicant in the exposure vessels must be constant and verified by measurements rather than calculated or measured only in stock solutions. Tests will generally be considered unacceptable if more than 10% of the toxicant is lost during the test.

- Test end points and lengths of exposure must be appropriate to the life stage of the species tested and the characteristics of the substance. Although the definitive bench mark for chronic toxicity is a whole life cycle test, partial life cycle and short term or early life stage tests are acceptable as chronic data (McKim, 1977). An example of this type of test is the fathead minnow, 7 day growth test (Norberg and Mount, 1985).

- Relevant environmental parameters such as temperature, pH and hardness must have been recorded.

- Responses and survival of controls must be appropriate for the species and test used.

Data on vertebrates and invertebrates not meeting all of the above are denoted as secondary in objective development documents. Secondary data are inadmissible in the development of a PWQO, but are listed and discussed in the PWQO development documents.

### 2.2.3 Minimum Data Requirements

The goal in setting PWQOs is to protect all forms of aquatic life. It is essential, therefore, to ensure that the Objectives are based on toxicity tests representative of a wide variety of life forms. The data must include vertebrates, invertebrates and plants and must consider the most sensitive lifestages.

PWQOs must be derived from literature conforming to the following rules for minimum data (additional minimum data requirements are also found in Sections 2.2 and 2.3 dealing with bioaccumulation and mutagenicity, respectively).

**FISH**

- Toxicological data from at least three different species including at least one cold-water fish species (e.g. Rainbow trout) and one warm-water fish species (e.g. Fathead minnow) must be present.
- At least one fish species must be resident in Ontario.
- Marine or brackish water species must not be used.
- The data must include two different chronic whole organism responses, and at least one of these must involve an early life stage.
- Acute lethal responses are generally not used except where a convincing case can be made that they are indicative of chronic lethality. For example, such data may be useable if a plot of LC50 values clearly showed than lethality had ceased well before the end of the test period.

**INVERTEBRATES**

- At least two different orders of invertebrates must be represented, one of which must be from the class Crustacea.
- Marine or brackish water species must not be used.
- Data from no more than one tropical invertebrate species may be used.
- Data must include two different responses and at least one of these must involve an early life stage.
- Acute lethality data are generally not used except when a convincing case can be made that acute lethal responses are indicative of chronic lethality. For example, acute lethality data may be useable if a plot of LC50 values at exposures less than 48 hours clearly showed that lethality had ceased before the end of the test period.

**ALGAE/AQUATIC PLANTS**

- At least one algae or aquatic plant species must be represented.
- Algae/plants must be freshwater species resident in temperate North America.

When assessing the aquatic impacts of phytotoxic substances (e.g. herbicides), special data requirements may be considered for algae and aquatic plants.

For any given substance, if the toxicological data available do not meet the minimum requirements, an Objective cannot be set and the process reverts to Guideline setting as described in Chapter 3.

### 2.2.4 Modifying Factors

Frequently the available toxicological literature indicates that factors such as water hardness, pH or temperature clearly modify the effects of a substance on aquatic life. Where the data for such a relationship are sufficiently clear, Objectives will be developed as a function of these modifying parameters. In these cases, the PWQO is expressed as a table of numbers and/or an equation defining the Objective at various levels of modifying parameters (i.e. ranges expected to occur in Ontario).

When modifying factors must be considered, it becomes more complicated to

define minimum data requirements. Generally, the available data should support the Objective in the ranges of the modifying parameters that are included in the table.

### 2.2.5 Safety Factors

A preliminary Objective is calculated based on the aquatic toxicity data. As long as the minimum data required to establish an Objective exist for a given substance, the lowest water concentration (including primary acute and chronic end points) causing significant responses is divided by a safety factor to obtain a preliminary Objective value.

The "safe" concentration may be different to protect against growth effects than it would be to protect against other toxic effects. Therefore, since all types of undesirable effects need to be prevented, the safety factor should account for relationships among concentrations causing various types of responses that could be observed for a substance. The minimum data requirements for establishing a PWQO cover this concern in part since there is a requirement to include at least one vertebrate and one invertebrate early life stage test. Early life stages are known to generally exhibit the most sensitive end points. Even with this consideration, however, there needs to be some safety factor to account for variation due to end points and for those cases where the early life stage is not the most sensitive.

The safety factor should also protect sensitive species that are not feasible to use as bioassay test organisms. Bioassay test species are not necessarily the most sensitive in aquatic environments. They are chosen partly because they are robust enough or are well enough known to be cultured in the laboratory. Inter-species differences in sensitivity to a toxicant are generally greater than are intra-species differences.

A margin of safety is also needed to account for the fact that laboratory animals are generally in better condition than are those in the field since they are fed daily under optimum conditions. Field animals are often under the stresses of winter fasting, parasites, predators etc. It is true that there is greater genetic diversity in the field allowing survival of the population in changing environments. However, since the Objectives are intended to protect individuals as well as populations, a safety factor is needed to account for the relative sensitivities of field versus laboratory-reared individual animals.

Few comparative studies exist that would assist in estimating these differences in sensitivity to a substance due to differences in species, end points etc. (e.g. Benoit *et al.*, 1982; Mayer *et al.*, 1986). The existing water quality criteria development documents are additional sources of comparative information. **A safety factor of 10 applied to the lowest effect concentration is used for setting the preliminary Objective value based on toxicity.**

### 2.2.6 Selecting a Preliminary Objective Value

These initial steps in developing an Objective, based on acute and chronic toxicity, are summarized as follows:

- A review of the world literature on acute and chronic toxicity is prepared for the substance.
- The available information is critically assessed to determine whether it is

acute or chronic, and primary or secondary data.

- If an adequate amount of primary information exists, the preliminary Objective is recommended at the lowest observed effect concentration divided by 10.

## 2.3 Bioaccumulation

Potential effects that may occur at the upper trophic levels in the food chain, from the consumption of contaminated biota, are not considered in the initial assessment involving toxicity. A separate assessment of bioaccumulation in the PWQO development process is therefore required. Regardless of whether bioaccumulation is the determining factor in setting the final PWQO value for a substance, a minimum amount of information is required for the assessment (Figure 2).

If both a reliable laboratory determination of body burdens in fish exposed to a known water concentration [i.e. a bioconcentration factor (BCF)] and information on the potential health effects in predators and/or human consumers of contaminated biota (generally these values are fish consumption limits endorsed by a recognized environmental or human health protection agency) are available, then a preliminary Objective based on bioaccumulation can be determined. This calculation is described in Sections 3.3.1 through 3.3.4.

If information on consumption limits is not available a preliminary Objective based on bioaccumulation cannot be set.

However, if reliable information suggests that BCF is less than 1000, bioaccumulation is not considered significant and the calculation of a preliminary Objective based on bioaccumulation is not required.

If BCF is greater than or equal to 1000, the whole assessment defaults to the Guideline setting process described in Chapter 3.

If no information on BCF is available, a measured octanol-water partition coefficient ($K_{ow}$) by a recognized method or, if reliable, a calculated $K_{ow}$ will be considered. For nonpolar organic compounds, the solubility in water is the primary physical-chemical property influencing the bioconcentration potential of a compound. The octanol-water partition coefficient is the most widely used quantitative measure of relative solubility properties (see Section 3.1 and Appendix A for a more detailed discussion).

It is assumed that substances with an octanol-water partition coefficient (log $K_{ow}$) of less than four do not bioaccumulate significantly and the calculation of a preliminary Objective based on bioaccumulation is not required.

If the log $K_{ow}$ is greater than or equal to four, or there are no data on $K_{ow}$, the whole assessment defaults to the Guideline setting process described in Chapter 3.

For metals, special considerations are needed on a case-by-case basis. Mechanisms of uptake and storage of metals in aquatic life are diverse and strongly influenced by chemical speciation and interactions with complexing ligands.

### 2.3.1 Consumption Guidelines

The BCF must be based on a controlled laboratory exposure in which the water

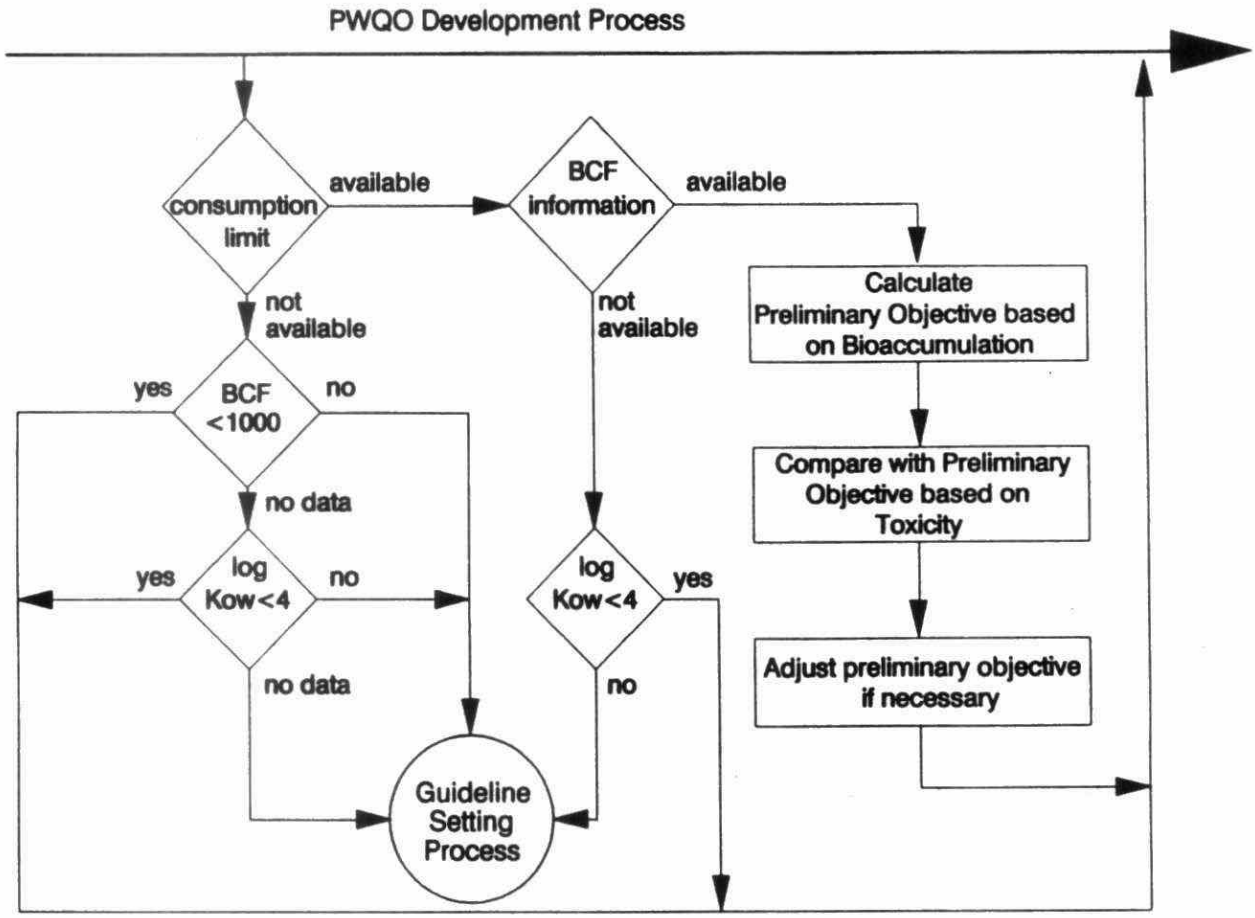


Figure 2. Bioaccumulation assessment for the PWQO development process

concentration was measured, the substance was bioavailable and present at less than known toxic levels. The BCF must be determined on a wet weight basis at steady state equilibrium. It must also be normalized for a lipid content of 10% as follows:

$$BCF = \frac{C_t}{C_w} \times \frac{10}{\%\ \text{lipid}}$$

where $C_t$ is the concentration in whole fish and $C_w$ is the water concentration.

A lipid concentration of 10% was chosen as a relatively high value to be protective. If more than one reliable BCF value is available, the highest value is used.

Fish consumption guidelines designed to protect human health or wildlife from the effects of eating contaminated fish are employed to define acceptable fish concentrations.

Fish consumption guidelines are developed by Health and Welfare Canada or similar health protection agencies (e.g. U.S. Food and Drug Administration,

World Health Organization). If more than one consumption limit is available, the value endorsed by Health and Welfare Canada is given preference and is used to calculate the concentration for determining the preliminary Objective based on bioaccumulation.

### 2.3.2 Fish Equivalency Concentration

Unfortunately, fish consumption limits are not available for many substances. The following may assist in developing surrogate limits from related information. Caution must be exercised, particularly if the bioaccumulation calculation determines the final PWQO.

If an allowable daily intake (ADI) value is available, a fish equivalency concentration (FEC) can be calculated. Fish equivalency concentrations are not consumption guidelines. They are used in this process as a gross surrogate to address bioaccumulation concerns. Fish equivalency concentrations for organic chemicals are calculated to protect a 70 kg sport fish consumer. This is done by calculating a total allowable daily intake for the chemical in question. This allowable daily intake is converted to a chemical concentration in the edible portion (muscle fillet) of fish by allotting 50% of the ADI to fish and dividing this value by 25 grams, the average daily fish consumption by an angler in Ontario, (Cox *et al.*, 1989). For example, with an ADI value for a chemical pollutant of concern of 1 ug/kg body weight per day, a fish equivalency concentration of 1.4 ug/g is derived by substituting the appropriate values into the following equation:

$$FEC = \frac{(ADI \times 70\ kg \times 0.5)}{25\ g\ fish/day}$$

where FEC is the fish equivalency concentration.

### 2.3.3 Determining the Acceptable Water Concentration

There is currently a lack of information on which to base ambient water concentrations to protect wildlife from the deleterious effects caused from consuming contaminated fish. The Aquatic Criteria Development Committee is currently developing procedures to establish fish contaminant residue limits for the protection of predacious fish and wildlife. Until these limits are developed, the contaminant residue limits of the International Joint Commission and the non-carcinogenic based limits of the New York State Department of Environmental Conservation (Newell *et al.*, 1987) may be directly substituted into the equation as the whole fish concentration to calculate an acceptable water concentration.

It has been observed that the concentrations of organic chemicals in whole fish are approximately 2.5 times higher than those in the edible portions (Niimi and Oliver, 1983). If bioaccumulation factors represent the ratio between the concentration of a chemical contaminant in whole fish and the concentration in the exposure water, consumption limits must be expressed on a whole fish basis. Therefore, the fish consumption limit or the FEC is multiplied by 2.5 to convert this value to an acceptable concentration in whole fish. A water concentration designed to limit bioaccumulation in fish to meet the fish consumption guidelines is calculated by dividing the whole fish concentration by the lipid normalized bioconcentration factor (BCF).

$$C_w = \frac{\text{whole fish concentration}}{\text{lipid normalized BCF}}$$

where $C_w$ is the water concentration.

### 2.3.4 Calculating the Bioaccumulation-Based Preliminary Objective

Maximum allowable body burdens in fish would theoretically result if the calculated ambient water concentrations to protect against effects caused by the accumulation of chemicals in aquatic biota were permitted. Since it is not desirable to reach a maximum acceptable residue level of a substance in fish on a consistent basis, a safety factor of 10 is applied to the calculated water concentration. The final water concentration based on BCF is compared to the preliminary Objective based on toxicity and if it is more stringent, the value based on bioaccumulation becomes the preliminary Objective.

### 2.3.5 Summary

In summary, the steps for setting a preliminary Objective based on bioaccumulation are as follows:

- Information is sought on laboratory derived BCF and consumption guidelines designed to protect consumers of fish. If these data are available, a water concentration can be determined.

- A preliminary Objective is set by dividing the lowest consumption guideline by the highest BCF value found in the literature and then dividing that value by a safety factor of ten (10).

- This preliminary Objective value is compared to the preliminary Objective calculated using the aquatic toxicological information, the more stringent of these two values is carried forward to the next step in PWQO setting.

- If consumption limits are not available or cannot be derived, a preliminary Objective based on bioaccumulation cannot be set. The next step, then, is to assess the available BCF data or, in its absence, the octanol-water partition coefficient (log $K_{ow}$).

- If the BCF is less than 1000 or, in the absence of BCF data, the log $K_{ow}$ is less than 4.0, bioaccumulation is not considered significant and the calculation of an Objective based on bioaccumulation is not required.

- If the BCF is greater than or equal to 1000 or, in the absence of BCF data, the log $K_{ow}$ is greater than or equal to 4.0, bioaccumulation is considered a significant factor to be addressed and the whole assessment then defaults to the PWQG setting process described in Chapter 3.

- If, by lack of data, BCF and the log $K_{ow}$ data are not known, the substance could, potentially, be of concern for bioaccumulation. Therefore, a PWQO can not be calculated. The whole assessment then defaults to the PWQG setting process described in Chapter 3.

In some parts of Ontario, subsistence fishing is an important use of lakes and rivers. Available ADI values may not offer adequate protection to year-round consumers of large volumes of fish. In applying PWQOs to waterbodies where subsistence fishing occurs, additional safety factors, determined on a site-specific basis, may be warranted.

## 2.4 Mutagenicity

The induction of mutagenic events and mutation related diseases in organisms as a result of their exposure to pollutants is a serious and undesirable effect. For the purposes of setting mutagenicity Objectives, it is assumed that genotoxic damage, mutations and mutation related diseases, which are measurable in microbial, plant, insect and mammalian systems, can also be measured in aquatic organisms. The potential effects of such exposure are mutagenicity related diseases, such as heritable mutations, birth defects or cancer.

If sufficient information is available, the preliminary Objective for mutagenicity will be set to protect aquatic organisms from the effects of mutagenic or genotoxic pollutants. The preliminary Objective for mutagenicity will be compared to the preliminary Objective based on toxicity or bioaccumulation. The most stringent of these values will be adopted for consideration as the final PWQO.

A mutagenic pollutant is defined as a chemical which possesses the ability to induce permanent and heritable genetic change at the cellular or whole organism level. A genotoxic pollutant is defined as a chemical with the ability to induce damage to DNA, to trigger DNA repair systems, to form DNA adducts, to induce damage and/or sister chromatid exchanges in chromosomes, or to induce mutagenic events.

The data used to set these Objectives will be derived from experiments using aquatic species exposed under appropriate conditions. These Objectives are not designed to protect the consumers of these aquatic species, for example humans, terrestrial mammals or fish-eating birds. Such concerns are addressed in other areas of the PWQO development exercise dealing with bioaccumulation and the consumption of fish (Section 3.2).

Setting Objectives for mutagenicity assumes that a no effect concentration for mutagens can be identified (Schaeffer, 1981). Justification for such a threshold model arises from the fact that for most organisms mutations occur naturally at a given background rate, as the result of errors in DNA synthesis and/or repair. When organisms are exposed to a mutagenic pollutant, the lowest observable effect level (LOEL) would be that concentration inducing an increase in mutagenic events to a frequency which is significantly greater than the background mutation rate. In setting mutagenicity Objectives, a practical goal is to reduce the mutagenic risk for aquatic organisms to this background mutation rate and not to some theoretical and perhaps unachievable lower level.

Consistent with the PWQO setting process for aquatic toxicity (Section 2.2), the LOEL and not the no observed effect concentration (NOEL) will be used to set the preliminary Objective based on mutagenicity concerns.

Objective setting for mutagenic chemicals will be based on data from acceptable tests employing aquatic organisms as test species. The lowest concentration of a mutagenic compound which induces mutagenic events exceeding the background level, in the most sensitive aquatic species, will be used as the critical value. This value will be adjusted by a safety factor to establish a mutagenicity Objective for that compound.

In the initial stage of the process, the mutagenic potential of the chemical is determined using all available mutagenicity data. Only chemicals which are identified as mutagenic or genotoxic will continue to the stage of setting preliminary Objectives or Guidelines for mutagenicity. If a substance is shown to be non-mutagenic, this component of the PWQO process will be terminated.

Mutagenicity Objectives will be set based on the data from a minimum of three primary mutagenicity studies conducted on whole aquatic organisms. The critical concentration, that is the lowest level inducing an mutagenic effect in the most sensitive aquatic species, adjusted by a safety factor, will be considered the mutagenicity Objective. If the mutagenicity data available for a chemical are insufficient to establish an Objective or, in the case where data are not available to determine the mutagenic potential of a chemical, then a Guideline for mutagenicity will be set. That process is described in Chapter 3.

### 2.4.1 Acceptable Data

All mutagenicity data from tests employing acceptable protocols may be used in determining the mutagenic potential of a chemical. Objectives for mutagenicity, however, will be set only on data derived from aquatic organisms. Since PWQO's are expressed in units of concentration in water (e.g. mg/L), the Objectives for mutagenic chemicals will be derived from experiments using suitable species exposed in aqueous solutions. This includes data derived from tests using aquatic vertebrates, such as fish and amphibians, aquatic invertebrates, such as crustaceans, as well as aquatic plants. Ideally data on the incidence of mutagenicity related diseases will be used, such as cancer or heritable mutations induced in aquatic organisms by an identified mutagenic compound. Data on the incidence of cellular mutations, DNA damage or chromosome damage in whole aquatic organisms are also acceptable. Data from tests using measured aquatic levels of the chemical would be most appropriate. Data from tests reporting only nominal chemical levels are also acceptable but these data are secondary. In addition, data derived from bacterial, yeast or algal tests, exposed in the absence of endogenous activation systems, are acceptable. Such microbial data are representative of in-vivo (intact) organisms in the aquatic environment.

Data derived from non-aquatic organisms, such as, rodents (mammals), are unacceptable for setting Objectives and Guidelines. Similarly, results from tests using cell tissue-culture or microbial tests requiring endogenous activation systems (such as S-9) are not acceptable. These two data types are excluded because neither measures an effect in intact aquatic organisms.

Only data from tests which expose organisms for a period of time permitting adequate cell division (two cellular generations) or DNA replication are acceptable. The process of DNA replication profoundly influences the development and expression of mutagenic events.

Only tests using fresh water organisms will be acceptable for setting mutagenicity Objectives. Data from tests using fresh water and marine organisms may be considered in Guidelines. Examples of acceptable tests and acceptable species are given in Appendix B.

### 2.4.2 Minimum Test Protocol Requirements

Only data from properly conducted tests will be used. Each test must contain adequate quality control checks including negative controls and appropriate positive controls. Each test must provide data at a minimum of five concentrations, preferably including one approaching the acutely lethal concentration. Tests must have sufficient replication of control and treatment groups to assure credible statistical analysis. Tests must be conducted over a sufficient dose range to permit definition of a concentration-effect relationship as well as demonstration of a no-effect and lowest-effect concentration level. Data from tests which do not meet minimum data requirements will not be used in the setting of Objectives but may be considered in the development of Guidelines.

A chemical will be considered mutagenic if it induces a significant, (tested statistically, ANOVA or other such test), concentration-related increase in mutagenic events. In addition the substance is considered mutagenic if two or more concentrations induce a significantly greater number of these events than the control. A chemical which does not induce a concentration-related increase in mutagenic events will be considered non-mutagenic.

### 2.4.3 Primary and Secondary Data

Tests on aquatic species which meet minimum test protocol requirements and which utilize constant, measured, and continuous (flow-through) concentrations of chemical, applied without a chemical carrier, in aqueous solution, will be considered primary. Static and renewal tests (i.e. static tests with replacement) will also be considered primary if it can be shown that chemical concentrations did not change appreciably (i.e. $\leq$ 10%) over the duration of the exposure.

Ideally primary data should also define the chemical's mode of action. Such data should identify the most prominent genotoxic end-point, the organ or tissue most affected, the physiological activation and detoxification pathways as well as the formation of DNA adducts with the chemical directly or its metabolically activated products.

Tests which utilize any of the following will be considered secondary and unsuitable for the setting of Objectives:

- Tests <u>not</u> employing accepted laboratory practices of exposure and environmental controls. While all tests must be evaluated on a case by case basis, those tests following published protocols of government agencies or standard setting associations are generally acceptable.
- Tests using nominal (i.e. unmeasured) chemical concentrations.
- Tests exposures with appreciably variable (decreasing) chemical concentrations (i.e. >10%).
- Tests using chemical carriers (solvents).

Only data classified as primary will be utilized to set Objectives. Guidelines may be set using data classified as secondary or primary.

### 2.4.4 Modifying Factors

If test conditions confound the outcome of the experiment, then the data should be considered secondary. Factors should be identified which may affect the con-

centration or integrity of the test chemical, such as the presence of light when testing a photosensitive chemical. Factors which may alter the sensitivity of the test organism, such as the use of a second chemical to induce detoxification or activation metabolic pathways, should be noted. In addition use of a second chemical as a promoter should also be noted.

If however, mutagenicity is a function of environmental variability, then the Objective may be a function of that variable. Modifying parameters which may influence the expression of mutagenic events or which may influence the condition of the test organism could include temperature, D.O., pH, or conductivity of the aqueous medium.

If specific information is available for effects such as those noted above, it is to be noted in the mutagenicity Objective development document.

### 2.4.5 Process for Setting Objectives Based on Mutagenicity

The process for setting Objectives based on mutagenicity consists of first determining the mutagenic potential of the substance and then calculating the Objective based on mutagenicity.

#### 2.4.5.1 Determining Mutagenic Potential

A minimal set of data is necessary to set mutagenicity Objectives. The process for setting such Objectives is outlined in Figure 3.

At the initial assessment level, data from experiments utilizing non-aquatic as well a s aquatic species are considered in order to screen for mutagenic properties. At this assessment level, relevant data would include the results of short-term bacterial tests, mammalian tissue-culture assays, mammalian whole organism tests, as well as tests with aquatic species.

If data from a minimum of two test systems, including tests for mutagenic as well as chromosomal damage end-points, clearly demonstrate a chemical to be non-mutagenic, mutagenicity Objectives will not be set. Objectives for that chemical will be based on other types of toxicological data.

Data demonstrating a chemical's ability to induce a mutagenic or genotoxic response in at least two test systems, are necessary to consider a chemical mutagenic and to initiate the setting of a mutagenicity Objective.

If both positive and negative mutagenicity data are available, the chemical will be regarded as either mutagenic or non-mutagenic based on weight of evidence and through consultation with MOE authorities.

If mutagenicity data are not available, or if confirmatory data from two test systems are not available, the chemical would be directed into the Guideline process.

#### 2.4.5.2 Setting Mutagenicity Objectives

To set an Objective, the chemical must be shown to be mutagenic or induce mutagenicity related diseases in aquatic organisms. With many chemicals, sufficient data may not be available to assess its mutagenicity in aquatic species. If data from experiments using aquatic organisms are not available, the chemical will be directed into the Guideline setting process.

In order to set an Objective, data must be available for at least three primary studies

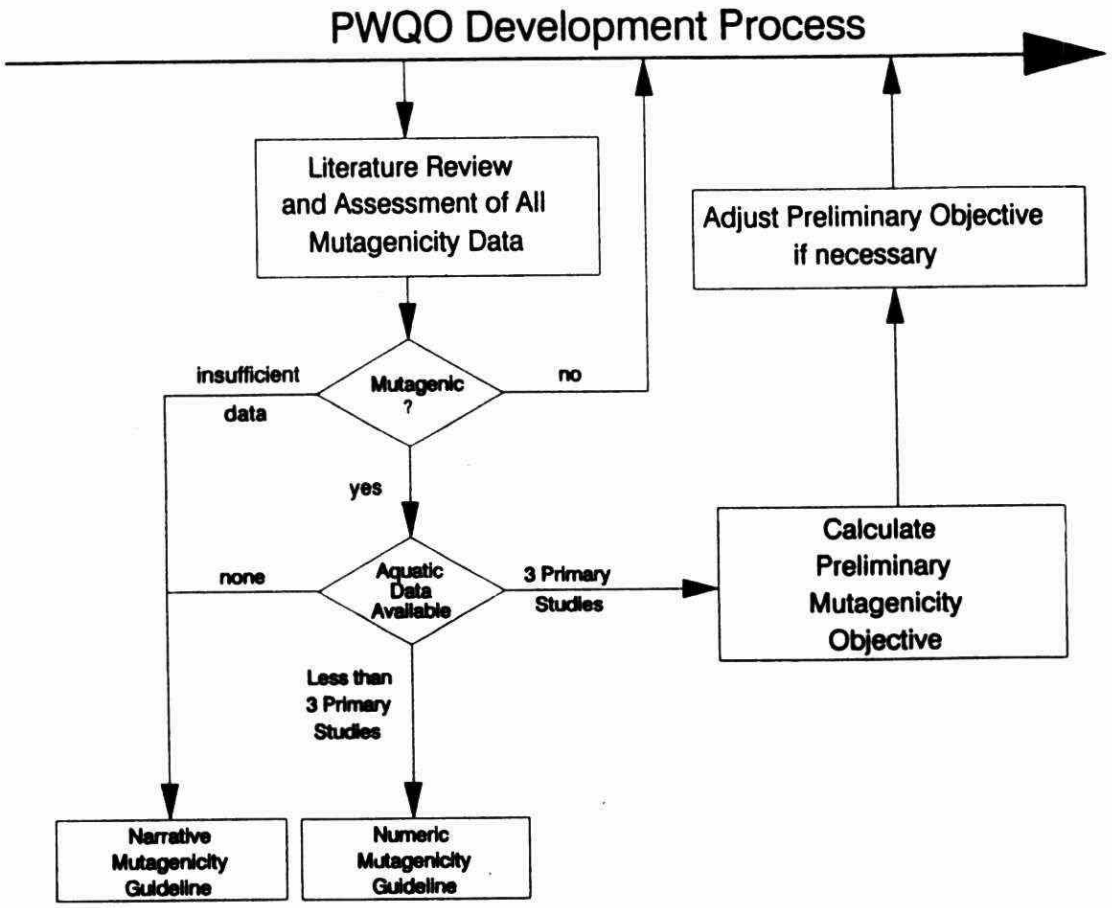


Figure 3. Mutagenicity Assessment for the PWQO Development Process.

demonstrating mutagenic events or mutagenicity related diseases in aquatic bacteria, plant, invertebrate or vertebrate species. Data need not be available for each level of organization (for example, three fish studies are acceptable for setting an Objective). However, the minimal data set must include results from at least one vertebrate study and must not include results from more than one plant or bacterial study. For each primary study, the lowest concentration inducing a measurable effect exceeding background [Lowest Observable Effect Level (LOEL)], would then be used in the Objective. The LOEL for the most sensitive aquatic species will be the critical value. This value is reduced by a safety factor to set a mutagenicity Objective.

### 2.4.6 Safety Factor

A safety factor will be used in the setting of mutagenicity Objectives. The use of this factor corrects for the possibilities that the most sensitive mutagenic or genotoxic end-point may not be measured in the available data. For example, tests measuring chromosomal damage may not detect additional genetic damage (such as

mutations) which may also be induced. In addition, the safety factor would add assurance in those instances where data from the most sensitive species are not available. Moreover, the sensitivity in detection of a mutagenic effect is dependent on the size of the population examined. The safety factor, accounts for the possibility that effects may be measured at lower concentrations of the chemical if larger numbers of organisms had been used in experiments. Finally a factor must be applied to account for variability in exposure-effect data experience within and between laboratories employing similar test procedures. To account for all uncertainties a factor of 10 is considered appropriate. **The lowest concentration of a mutagenic compound inducing a significant effect in the most sensitive species, is divided by a safety factor of 10 to establish a preliminary Objective for mutagenicity.**

### 2.4.7 Selecting a Preliminary Objective Value

The preliminary Objective based on mutagenicity is compared with the preliminary Objective based on toxicity or bioaccumulation, as described in Sections 2.2 and 2.3. The most stringent concentration of all the preliminary Objectives is then selected as the candidate PWQO.

### 2.4.8 Summary

In summary, the steps for setting a preliminary Objective for mutagenicity for the protection of aquatic organisms are as follows:

- A thorough search of the available mutagenicity test data is conducted.
- Only data from acceptable tests, employing acceptable test protocols, will be used.
- The substance is initially assessed for its ability to induce mutagenic or genotoxic damage in tests employing both aquatic and non-aquatic species.
- If a minimum of two data sets, which include tests for both mutagenic and chromosomal damage end-points clearly demonstrate (no positive data) the chemical is non-mutagenic, the mutagenicity Objective setting exercise is terminated.
- If data from two different test systems show mutagenic properties of the chemical, the chemical continues in the mutagenicity Objective setting process.
- If no data are available to assess its mutagenic properties, or if data from a single test demonstrates a chemical mutagenic but a second data set demonstrating mutagenic or genotoxic properties is not available, the chemical is directed to the Guideline setting process.
- In some cases where data are conflicting, indicating both mutagenic and non-mutagenic results, the chemical will be considered either mutagenic or non-mutagenic based on weight of evidence and in consultation with MOE authorities.
- If data from acceptable tests employing aquatic organisms are not available, or if fewer than three primary aquatic organism data sets are available, the chemical is directed into the Guideline setting process.

- If a minimum of three primary, aquatic organism data sets are available, the LOEL (lowest concentration inducing a measurable mutagenic effect) for each data set is summarized. The LOEL for the most sensitive aquatic species is selected as the critical value.

- The critical LOEL value is divided by a safety factor of 10 to set the mutagenicity Objective.

- This preliminary Objective for mutagenicity is compared with the preliminary Objective based on toxicity and bioaccumulation. If the mutagenicity Objective is the most stringent concentration, then this value is carried forward to the next step in the PWQO setting.

## 2.5 Impacts on Taste and Odour in Water and Tainting of Fish Tissues

To adequately protect the recreational uses of surface waters of the province, PWQOs must ensure the natural quality of these waters are not impaired by the imparting of taste and odour in water and/or fish by chemical pollutants.

Odour in water, taste in water, and tainting (taste or odour) of fish tissue which may affect its palatability are effects that can clearly influence the quality and thereby impact on the recreational use of surface water (i.e. fishing, swimming, bathing etc.). The data required for Guideline setting are normally obtained through a review of pertinent literature. These data should be derived from properly designed experiments with measured concentrations of, at least, the stock solutions of chemical (Amoore and Hautla, 1983). Taste and odour effects of substances in water should be obtained with water temperatures of 30° C or less. Tainting values are expressed as water concentrations that result in taste or odour in the fish tissue.

Threshold concentrations eliciting an odour or taste in water or an off-flavour or odour in fish-tissue may be used to set a preliminary Objective. While the MOE is not requiring strict adherence to any specific protocol for the admissibility of such data, there are some fundamental conditions that must be met if the data are to be used:

**Fish Tainting**

- Fish used in the test should be exposed to the substance for a minimum exposure time of 48 hours before being sacrificed and prepared for the taste panel.

- The dilution series should elicit a range of responses from strong to no response.

- Panels should consist of at least six people, preferably non-smokers.

- Taste testing should be carried out in an odour-free room (preferably with filtered air).

- Precautions should be taken to ensure no loss of chemical during testing of volatile chemicals.

**Taste and Odour of Water**

- Dilution series should range from strong response to no response.

- A panel size of 20 non-smokers is desirable although a minimum panel size of six is acceptable.

- Dilutions of test compounds must be prepared using odour-free water (preferably obtained by passing water through an activated carbon filter).

- Taste and/or odour testing should be carried out in an odour free room (preferably with filtered air).

- Since warm water may taste unpleasant, the samples should be presented at room temperature for judgement of taste.

- When judging the odour of a chemical in water, the temperature of the solution should not exceed 30° C.

If an effect concentration is below or just above (i.e. within an order of magnitude) the preliminary Objective, based on aquatic toxicity, bioaccumulation or mutagenicity, special attention should be given to identifying the best available effect concentration.

Because fish tainting and taste or odour of water are expressed as threshold water concentrations that can be perceived by people with sensitive olfactory senses, a safety factor of two (2) was arbitrarily selected to calculate a "no-effect" level or taste/odour protection value.

If the value calculated from the assessment of impacts on taste and odour in water and tainting of fish tissues is more stringent than the preliminary Objective value calculated from toxicity, bioaccumulation or mutagenicity, then this value is carried forward to the next step in the PWQO setting.

## 2.6 Recreation

Traditionally, the Objectives for the protection of recreational water uses have been based on public health concerns (e.g. microbiological contamination, eye irritation) and aesthetic considerations (e.g. colour, clarity). Procedures for the development of such Objectives tend to be issue specific.

In setting PWQOs for recreational use, the principal concern relates to the impact of chemical substances on humans during recreational uses of water through direct dermal exposure or accidental ingestion of water while swimming or during similar recreational activities. At this time, the Ministry is unable to make conclusive assessments on the risks to bathers through such pathways but will continue to evaluate procedures for directly assessing recreational use requirements in PWQO setting activities.

Should information on recreational uses of water be found during the literature search, it will be documented and assessed.

## 2.7 Wildlife Protection

The protection of wildlife is also a consideration when setting a PWQO. Some wildlife occupy niches that can potentially expose them to elevated levels of contaminants in the aquatic environment. Those that rely on aquatic environments and particularly those birds (e.g. osprey, gulls, etc.) and mammals (e.g. mink) that consume large quantities of fish and other aquatic organisms are at greatest risk.

The health significance of residue levels within aquatic organisms is currently under study by MOE. Substance-specific

guidelines will be set for permissible residue levels. Procedures will then be established for relating these guidelines to PWQO values.

Where appropriate data on BCF and acceptable intake levels are available, the protection of fish-eating birds or mammals is addressed by considering bioaccumulation (Chapter 2.3).

No specific procedures are yet in place for evaluating proposed PWQO values in relation to the health of wildlife drinking the water. Any relevant information found during the literature review phase is assessed on a case by case basis for possible use in adjusting the PWQO.

## 2.8 Sediment Quality

Contaminants in sediment are a concern because of their potential effect on overlying water quality and water use, their impact on abundance and community composition of the benthic community and their effect, through bioaccumulation, on the organisms higher in the food chain which feed on benthos.

Work is underway to develop a set of guidelines for sediment quality. They would represent a desirable level of sediment quality the Ministry strives to maintain in sediments of the Province.

Because of the links between sediment quality and water quality, proposed PWQOs should be evaluated to determine their potential effect on sediment quality. As sediment quality guidelines become available, these evaluations can be made.

## 2.9 Other Effects

The Objective setting process does not explicitly address or consider interactions with other contaminants (e.g. synergistic toxicity), ecological effects, sediment loading, wildlife protection or recreational water uses. However, it is felt that the use of conservative safety factors will result in an Objective that should afford adequate protection for most other beneficial uses of surface waters, with the exception of drinking water supplies which are addressed directly through the Ministry's Drinking Water Objectives. Where available data permit, Objective values can be related to physical and chemical parameters such as water temperature, pH, and hardness. If specific information is available for effects such as those noted above, it is provided in the Objective development document.

## 2.10 Recommending the Final PWQO

The most stringent of the preliminary Objectives developed in the preceding sections of the document is recommended as the PWQO.

## 2.11 Objectives of Other Agencies

Where available, aquatic environmental criteria of other agencies are to be noted and discussed in the PWQO development document (e.g. CCREM, 1987). Although the criteria of other agencies are not used to alter the PWQO, since the other agencies have different procedures and strategies, they provide a useful comparison.

## 2.12 Research Needs

Any special data requirements which would contribute to improving the PWQO should be identified (see Table 6).

# 3 SETTING PROVINCIAL WATER QUALITY GUIDELINES

The Ontario Ministry of the Environment recognizes the need for a procedure to derive water quality guidelines for environmental contaminants where data on aquatic toxicity, mutagenicity and bioaccumulation are insufficient for the development of Provincial Water Quality Objectives. The procedure described in this chapter provides a rational method for consistent development of Provincial Water Quality Guidelines (PWQGs) for organic and inorganic pollutants.

A preliminary Guideline value is calculated by applying a safety factor (called a final uncertainty factor) to the lowest water concentration shown to cause a toxic effect. Since the available database on aquatic toxicity varies from substance to substance, so does the level of assurance in the final product (i.e. the PWQG). In order to account for this and ensure environmental protection, a specific uncertainty factor is calculated for each substance. The size of the uncertainty factor is determined by the physical-chemical properties and the quality and quantity of the aquatic toxicity database.

Although Guidelines and Objectives serve the same purposes, the following points must be kept in mind:

- Guidelines are not as scientifically supportable as PWQOs because they lack the comprehensive data base required for the derivation of Objectives.

- The intention of the Guideline derivation process is to ensure consistency in the interpretation and use of data for setting numerical values and to develop the best possible recommendation based on available data.

- As new data become available, Guidelines will be periodically reassessed and, if warranted, modified using the Ministry's PWQO setting process. The Guideline setting process requires identification of the scientific research needed to support this step.

## 3.1 Substance Physical-Chemical Properties

The fate and effects of organic contaminants in aquatic systems are largely determined by their inherent physical-chemical properties. Hence a knowledge of fundamental substance properties (e.g. molecular weight) is essential in any assessment of potential environmental effects (Klein *et al.*, 1988; Kobayashi, 1981; U.S.E.P.A., 1990). Where this information is available, it is recorded on the Physical-Chemical Properties sheet (Table 1 - Appendix C).

The most useful chemical properties are those which describe the equilibrium tendencies of a chemical to partition between the various phases (water, biota and sediment) present in an aquatic system. These properties are usually solubilities, vapour pressures or partition coefficients. They may include information about dissociation or speciation of the chemical.

A key property in this regard is octanol-water partition coefficient ($K_{ow}$). $K_{ow}$ is the ratio of chemical solubility in octanol (a nonpolar phase) to solubility in water (a polar phase). Nonpolar organic chem-

icals with a high log $K_{ow}$ (>4) accumulate and reside in nonpolar phases of the environment such as the fatty or lipid-rich tissues of aquatic organisms. Since chemical affinity for octanol is reasonably well correlated with affinity for lipids, octanol has become, for environmental applications, a useful surrogate or model nonpolar organic phase.

It is generally accepted that substances with high $K_{ow}$'s have significant potential to persist and accumulate in aquatic biota, reaching concentrations which could pose a direct threat to aquatic life and to wildlife and humans consuming aquatic species (Alexander,1981; Niemi, 1987; Veith *et al.*, 1988; Connell, 1990).

Well-known contaminants such as mirex and DDT are examples of substances with high octanol-water partition coefficient values which persist in the environment and accumulate in biota.

Values for $K_{ow}$ are commonly obtained by measurements using equilibrium shake-flask methods or chromatographic retention times (De Bruijn *et al.*, 1989; Doucette and Andren, 1988; Veith *et al.*, 1979). Where a measured value is unavailable, a $K_{ow}$ value can be estimated using correlations with chemical structure or equilibrium properties (Lyman *et al.*, 1982; Miller *et al.*, 1985). Other procedures for *a priori* calculation of an unknown $K_{ow}$ value are outlined in Hansch and Leo (1979) and Lyman *et al.* (1982). Note that calculation of $K_{ow}$ can be quite complex and measured values are preferred.

$K_{ow}$ values are available in the literature for most of the substances which are candidates for Guideline setting (De Bruijn *et al.*, 1989; Doucette and Andren, 1988; Hansch & Leo, 1979; Leo *et al.*, 1971; Lyman *et al.*, 1982; Veith *et al.*, 1979). In many cases, the variation between reported values is substantial, especially in the high $K_{ow}$ range where measurement of $K_{ow}$ is difficult and calculated values are often overestimates.

## 3.2 Selection Of Baseline Uncertainty Factor

If available information indicates that a BCF has been reliably determined for a substance in a species of fish, the preliminary Guideline based on toxicity is calculated using a baseline uncertainty factor of 1000 for a BCF of less than 1000 (whole body basis) or a baseline uncertainty factor of 10,000 for a BCF greater than 1000.

If this information is unavailable, $K_{ow}$ values are used in Guideline development to select an initial uncertainty factor called the baseline uncertainty factor which is the starting point in the Guideline setting process:

If log $K_{ow} < 4.0$, the baseline uncertainty factor = 1000

If log $K_{ow} \geq 4.0$, the baseline uncertainty factor = 10,000

While these baseline uncertainty factors and the calibration factors (See Table 4) were arbitrarily selected values, their derivation was based on the fact that the PWQG for a substance with a log $K_{ow} < 4.0$ and a complete data set would have a final uncertainty factor slightly greater than 10 (See Section 2.2.5).

Where both a measured and estimated or calculated $K_{ow}$ value is available, the measured value is selected as the final value on Table 4 (Appendix C). Al-

though an accurate value for $K_{ow}$ is desirable, selection of the baseline uncertainty factor depends only on a determination that log $K_{ow}$ is less than or greater than four. If log $K_{ow}$ is unknown, or if a substance has a range of values spanning log $K_{ow}$ = 4.0, select 10,000 as the baseline uncertainty factor.

Inorganic forms of metals are assigned a baseline uncertainty factor of 1000.

## 3.3 Evaluation of Toxicological Data

A scientific assessment of the toxicity test data must be documented in the Guideline report, with special attention given to the studies from which the lowest observed effect concentrations were obtained. All relevant data from toxicity tests, including test conditions, obtained from the literature review, must be listed on the Aquatic Toxicity Data Table (Table 2). Toxicity values (e.g. LC50s) are also plotted on the Guideline Derivation Graph (Figure C1). The toxicity value which is the lowest observed effect concentration must be highlighted on both the table and the graph. When necessary, the toxicity values may be plotted as ranges to conserve space on the graph.

### 3.3.1 Primary Or Secondary Data

Guidance for categorizing data as acute or chronic and primary or secondary is provided in PWQO Section 2.1.2. Standard test procedures or protocols do not always generate primary data. Therefore, best scientific judgement must be used to justify a primary or secondary designation for toxicity data, on a case by case basis.

### 3.3.2 Optimal Data Requirements

All available aquatic toxicity data on a substance are reviewed to determine the lowest water concentration associated with an adverse biological effect. However, only different types of information, up to a maximum of 11 toxicity values, qualify for the determination of the final uncertainty factor. These types are designed to represent a range of acute and chronic biological effects in a variety of aquatic species.

The following list indicates the optimal data requirements for use in setting Guidelines (Table 3):

**CHRONIC DATA ON:**

- Three different species of fish.
- Two invertebrate species from different orders.
- One algal or aquatic plant species.

**ACUTE DATA ON:**

- Three fish species.
- Two invertebrate species representing different orders.

Toxicological data on marine or brackish water species may not be used in the Guideline setting process.

Data on the aquatic life stage of amphibians can be substituted, appropriately, for one of the six possible fish data listed above.

Data on the aquatic life stage of protozoa can be substituted, appropriately, for one

of the four possible invertebrate data listed above.

### 3.3.3 Simulated Data

Toxicity data simulated by quantitative structure-activity relationships (QSARs) and acute-chronic ratios (ACRs), which meet the requirements, for different species may be used to a limited extent where measured toxicity data are not available. Information on these data simulation approaches is provided in (Bobra *et al.*, 1985; Call *et al.*, 1985; Könemann, 1981; McCarty *et al.*, 1985; Veith *et al.*, 1983; Kenaga, 1982; Richter *et al.*, 1983) and Appendix A.

In Using Simulated Data the Following Rules Apply:

- A QSAR equation may be used once in Guideline setting to interpolate a species-specific simulated acute toxicity value for a compound within the chemical class to which the QSAR applies.
- An ACR, derived from a study designed to establish this ratio, may be applied once to an acute toxicity value for a second fish species to calculate a simulated chronic toxicity value.
- Simulated toxicity values may be used in the absence of measured data to contribute to a decrease in the final uncertainty factor and are plotted on the Guideline Derivation Graph. In the case of ACR's, the acute value used to set the chronic value from the ACR is not used again at later stages in the Guideline setting process.
- Simulated data cannot be employed as the critical data point to which the final uncertainty factor is applied.

### 3.3.4 Application of Toxicological Data

Each toxicity value up to a maximum of 11, which qualifies as a different type of information is now assigned a calibration factor (listed in Appendix C) according to the data categories to which it was assigned; i.e. acute or chronic and primary or secondary. Calibration factors are multipliers applied to the baseline uncertainty factor to calculate a final uncertainty factor. They represent the weight or influence of the information in reducing baseline uncertainty and provide the link between the quality and quantity of available toxicity information and the size of the final uncertainty factor. Toxicity data are the primary determinants of the final uncertainty factor.

Specific values for the calibration factors were selected so that a data set of primary acute and chronic test results for fish, invertebrates and aquatic plants would produce a final uncertainty factor compatible with the existing safety factor used in PWQO development. Calibration factors for secondary data and plant data were determined by discounting the calibration factors which were so selected.

In order to obtain consistency between chemicals, the Guideline setting process must be strictly followed with very little deviation from the prescribed methods. The calculation of a preliminary Guideline is documented on the Toxicity Guideline Uncertainty Factor Worksheet (Table 4). The steps are as follows:

1. Determine the octanol-water partition coefficient, $K_{ow}$ and use the log $K_{ow}$ value to select the baseline uncertainty factor indicated on Table 1. Re-enter the baseline uncertainty factor at the bottom of Table 4.

2. Enter in the boxes on Table 4 the key data on each toxicity test.

   If more than one test result has been categorized as the same type of information (e.g. if there are three 96h-LC50s for rainbow trout), preference for inclusion on the form should be given to the test results which have been assigned the lowest calibration factors (i.e. primary over secondary data and measured over simulated data).

   Data which yield the lowest final uncertainty factor should be used on the uncertainty factor worksheet (Table 4). **The lowest observed toxic effect concentration (i.e. the critical value) need not be entered in one of the boxes on the uncertainty factor worksheet (Table 4), even though it is used in the calculation of the preliminary Guideline.**

   If there are unfilled acute data boxes, unused chronic data may be used in these boxes provided other requirements (i.e. species diversity) are met. The extra data are considered, for the purpose of reducing uncertainty, as useful as acute information and are entered and assigned a calibration factor for acute information.

   If all data boxes cannot be filled, one simulated acute and/or one simulated chronic toxicity value may be used.

3. Re-enter the calibration factor associated with each test result at the bottom of Table 4. Multiply the baseline factor by all the calibration factors to determine the final uncertainty factor. The final uncertainty factor is not to be less than a value of 13.

4. To calculate a preliminary Guideline value, divide the lowest observed toxic effect concentration by the final uncertainty factor.

**The minimum data requirement to set a Guideline is one piece of toxicity data (e.g. an LC50 value), acute or chronic, primary or secondary, for a fish or invertebrate.** Guidelines cannot be based only on plant, amphibian, protozoan and/or simulated data alone.

A preliminary Guideline based on aquatic toxicity data may be superseded by consideration of other effects described in the following sections.

## 3.4 Bioaccumulation

Information on both bioaccumulation and consequent health effects is unlikely to be available for the vast majority of industrial organic contaminants. The Guideline setting process considers this limitation and permits the calculation of a Guideline which acknowledges concerns about bioaccumulation. This is done initially through the selection of the baseline uncertainty factor based on a reliably determined BCF or the octanol-water partition coefficient (See Section 3.2 and Figure 2).

If scientifically sound data on bioconcentration and health effects are available, the information is used to calculate a preliminary Guideline as outlined for PWQOs (Section 2.3) and compared to the toxicity-derived Guideline. The lower value would then be recommended as the final PWQG. If bioaccumulation data determine the Guideline, the study used to derive the BCF must be thoroughly investigated and documented in the final report.

## 3.5 Mutagenicity

A mutagenicity Guideline will be set when sufficient primary information is not available to set a PWQO based on mutagenicity concerns or when there is insufficient data to assess the mutagenic potential of the chemical. The data requirements to set a mutagenicity Objective or to consider a chemical non-mutagenic are presented in Section 2.4.5.1.

A chemical clearly shown to be non-mutagenic need not be assessed further in either the mutagenicity Objective or Guideline process.

Only acceptable data, as outlined in Mutagenicity Objective Section 2.4.1, with the minimum test protocol requirements, as outlined in Section 2.4.2, will be used in setting these Guidelines. However, this Guideline process will consider both primary and secondary data as defined in Section 2.4.3. In addition data from tests using marine organisms may be considered as secondary data in setting mutagenicity Guidelines but not in Objectives.

In many instances primary studies will not be available. In such cases, the available primary information, in combination with any available secondary information will provide the data for setting a mutagenicity Guideline. However, Guidelines will not be set based solely on the results of microbiological or algal studies.

In the case of mutagenicity Guidelines, simulated data derived from QSAR studies will not be used.

The circumstances which require a chemical to be considered in the Guideline process for mutagenicity are identified in Section 2.4.5. Depending on the availability of acceptable data, a narrative or numeric mutagenicity Guideline may be set. A narrative Guideline will only be set when there are insufficient data to either assess mutagenic potential or to set a numeric Guideline for aquatic organisms.

### 3.5.1 Numeric Mutagenicity Guidelines

Numeric Guidelines may be set when acceptable data, either primary or secondary are available from tests using aquatic organisms. Only data meeting the minimum requirements will be considered. Available mutagenicity data are summarized, and the pertinent information entered into Table 5 (Appendix C).

If available information indicates that a BCF has been reliably determined for a substance in a species of fish, the preliminary Guideline based on mutagenicity is calculated using a baseline uncertainty factor of 1000 for a BCF of less than 1000 (whole body basis) or a baseline uncertainty factor of 10,000 for a BCF greater than 1000.

If this information is unavailable, a baseline uncertainty factor is chosen based on the log $K_{ow}$ as follows:

If log $K_{ow} < 4.0$, the baseline uncertainty factor = 1000

If log $K_{ow} \geq 4.0$, the baseline uncertainty factor = 10,000

This value is entered into Table 5.

The use of an uncertainty factor of 10,000 for mutagenic chemicals with a BCF$\geq$ 1000 or a log $K_{ow} \geq 4$ is based on potential accumulation of the chemical in the aquatic food chain by organisms incapable of metabolizing or excreting the chemical. Predators having the ability to metabolize

these chemicals could thus receive a much larger dose through the diet than through waterborne exposure alone.

#### 3.5.1.1 Optimal Guideline Data Requirements

The available acceptable data are sorted as primary or secondary studies, and aquatic vertebrate, invertebrate, plant or microbial organism categories. The suitable studies fall into the following categories:

Primary data from either combination:

2 vertebrate species, and 1 plant species or microbial species

OR

1 vertebrate and 1 invertebrate species, and 1 plant species or microbial species

Secondary data from:

2 vertebrate species
2 invertebrate species
1 plant species
1 microbial species

The range of studies should include data demonstrating mutagenic and/or genotoxic end points as well as whole organism effects such as heritable mutations or carcinogenicity (for mutagenic carcinogens). In addition, attempts should be made to obtain data from organisms which can and cannot metabolize the chemical.

For each selected study the LOEL values are summarized on Table 5 (Appendix C). In addition, each study is assigned a calibration factor, as outlined in the Legend, on the basis of primary or secondary data classification. Within organism categories, data from the most sensitive species will be used.

The baseline uncertainty factor is multiplied by all the calibration factors to determine the final uncertainty factor.

The preliminary mutagenicity Guideline for the chemical is calculated. The mutagenicity LOEL value for the most sensitive species from all organism categories is selected as the critical value. This LOEL value is divided by the final uncertainty factor to determine the preliminary Guideline based on mutagenicity for that chemical. If this value is more stringent than the preliminary Guideline determined for toxicity and for bioaccumulation, then this value is carried forward to the next step in PWQO setting.

### 3.5.2 Narrative Mutagenicity Guidelines

A chemical which has not been tested for genotoxic properties or which has not been tested in aquatic organisms may be given a narrative Guideline. Under these conditions the chemical will remain in the Guideline process until data become available and will include one of the following cautions:

a) No mutagenicity data available.

- for chemicals which have not been tested for mutagenic or genotoxic activity in any system.

b) Insufficient data to confirm mutagenicity.

- for chemicals shown to be mutagenic or genotoxic in a single acceptable test but which have been shown to be non-mutagenic or non-genotoxic

in all other available tests, or where no additional data are available.

c) Mutagenic - no aquatic data available.

- for chemicals which have been confirmed mutagenic in two tests with acceptable protocols, but where data with aquatic organisms are not available.

## 3.6 Impacts on Taste And Odour of Water And Fish Tissues

The acquisition, evaluation and use of data follows the same steps as outlined for PWQOs.

## 3.7 Other Effects

The Guideline setting process does not explicitly address or consider interactions with other contaminants (e.g. synergistic toxicity), ecological effects, sediment loading, wildlife protection or recreational water uses. However, it is felt that the use of conservative safety factors will result in a Guideline that should afford adequate protection for most other beneficial uses of surface waters, with the exception of drinking water supplies. Where available data permit, Guideline values can be related to physical and chemical parameters such as water temperature, pH, and hardness. If specific information is available for effects such as those noted above, it is provided in the Guideline development document.

## 3.8 Recommending the Final PWQG

The most stringent of the preliminary Guidelines developed in the preceding sections of the document is recommended as the PWQG.

## 3.9 Objectives of Other Agencies

Where available, aquatic environmental criteria of other agencies are to be noted and discussed in the Guideline document. These values should be plotted on the Guideline Derivation Graph. While the criteria of other agencies will not be used to alter the PWQG, they will provide a useful comparison.

## 3.10 Research Needs

A description of any data required to promote a Guideline to an Objective, such as acute or chronic toxicity data, BCF, octanol-water partition coefficient or mutagenicity data, should be provided. An example of the required data list (Table 6) is provided in Appendix C.

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## APPENDIX A – Bioaccumulation: Theoretical Considerations

Bioconcentration generally refers to the process by which an aquatic organism, when exposed only to water containing a concentration of chemical ($C_w$), absorbs the chemical from solution and accumulates a higher concentration ($C_b$) (McKim *et al.*,1985; Connell, 1988). The ratio $C_b/C_w$ is a bioconcentration factor (BCF). Bioconcentration can only be measured in the laboratory because there is, by definition, no exposure via consumption of contaminated food.

In general, BCF refers to a steady-state condition in which uptake and elimination (clearance) rates have equalized. If an organism cannot readily metabolize or eliminate the chemical compound, the steady-state corresponds to an equilibrium condition in which chemical transport by passive diffusion (exchange partitioning) is the prime determinant of BCF.

BCF may also be defined, for a simple fish-water system, as a ratio of uptake and elimination (first order) rate constants, $k_1/k_2$, respectively (Neely, 1979). Each rate constant quantifies the fraction of chemical absorbed or eliminated in unit time. They are determined, for a particular substance and fish, by measuring changes over time in the chemical concentration in biota observed in separate uptake and elimination experiments.

A review of empirical BCF data for a wide range of nonpolar organics suggests that uptake rate constants vary by a much smaller factor than do elimination rate constants and it is the latter which accounts for most of the differences in BCF between compounds (e.g. Könemann and van Leeuwen, 1980; Bruggeman *et al.*, 1981). In addition, the exposure time necessary to reach a steady-state equilibrium condition depends only on the elimination rate constant. Niimi (1987) provides a recent review and compilation of values of this key kinetic parameter.

In the ambient aquatic environment organisms may accumulate chemicals from both water and food; a process termed bioaccumulation. The ratio $C_b/C_w$ is, in this case, a bioaccumulation factor (BAF). If the concentration of chemical in food ($C_e$) is known, $C_b/C_e$ is sometimes referred to as a biomagnification factor (BMF). The relative importance of food as an exposure route to aquatic biota increases with increasing body size of the organism and increasing hydrophobicity of the chemical.

If experimental data on chemical disposition in aquatic biota were available, a pharmacokinetic model could be derived and used to assess bioconcentration potential. The available information is, however, insufficient to justify such a model. Given the large number of contaminants which have been detected in aquatic systems, it is unlikely that a comprehensive data set for each and every chemical will ever be available.

It is clear that a simple screening procedure is required. One which enables predictions or simulations to be made of relative bioaccumulation potential from a standard set of chemical benchmark properties; so-called partitioning models based on quantitative

structure-activity relationships (QSARs). The QSAR approach is a practical and consistent procedure which provides simple descriptors for:

1. *a priori* estimation of BCF from $K_{ow}$

2. extrapolation of measured BCF values for a given water-biota system to other biota or other structurally similar chemicals

3. evaluation of existing BCF data based on "expected behaviour"

For example, many linear relationships of the general form:

$$\log BCF = a \log K_{ow} + b$$

have been derived and reported in the literature. The slopes (a) and intercepts (b) of these linear correlations vary greatly for a variety of reasons, including both biological differences in test species (Barber *et al.*,1988) as well as experimental and statistical artifacts and errors (e.g. short exposure times, unconsidered chemical bioavailability and over-estimated $K_{ow}$ values). Any given set of values for the constants in this general equation are therefore specific to the test system from which the data were obtained.

It is not possible, at present, to easily separate or delineate all the factors which contribute to variations between correlations. One solution is to develop correlations based on compiled data sets, as has been done by Lyman *et al.* (1982). However these correlations tend to underestimate the bioaccumulation potential of persistent hydrophobic chemicals.

The following approach, based on simple fish-water exchange partitioning theory and key biological attributes, is recommended as an assessment tool:

The simplest analysis is based on the assumptions that an organism achieves equilibrium with water and that the lipid portion of the organism is equivalent in properties and amount to octanol. The chemical concentration in organism lipids ($C_l$) will then be the product $C_w \times K_{ow}$. For example, if the water concentration is 0.1 g/m$^3$ and $K_{ow}$ is 1000, then the concentration in the lipid will be 100 g/m$^3$. If the organism consists of 5% lipids (i.e. lipid volume fraction (L) is 0.05), then the whole body concentration ($C_b$) will be 0.1 x 0.05 x 1000 or 5 g/m$^3$. In general terms:

$$BCF = L \times K_{ow}$$

This type of analysis is generally satisfactory for compounds with: a high proportion of C-C (aliphatic), C-C (aromatic), C-H and C-Cl bonds, molecular weight <300 g/mol, molar volume <250 cm$^3$/mol, log $K_{ow}$ 1-6, water solubility 0.002-18 mol/m$^3$ (Connell, 1988). These structural attributes and physical-chemical properties are closely interrelated and generally describe nonpolar, moderately hydrophobic chemicals which are resistant to biotic and abiotic transformation (e.g. persistent chlorinated hydrocarbons).

There is, however, a loss of linearity in the BCF-$K_{ow}$ correlation at high $K_{ow}$'s, in both laboratory and field situations. There are at least eight possible reasons (both experimental artifacts and real phenomena) which must be considered when judging the validity and applicability of both measured and estimated BCF values:

1. If log $K_{ow}$ is low, i.e. less than 1 , the substance displays an almost equal tendency to partition between lipids and water. Bioconcentration will be underestimated because a significant fraction of the chemical will be present in the organism's water phase (Gobas, *et al.*, 1986). A convenient "correction", for the purpose of estimating BCF, is to add 1.0 to $K_{ow}$ (not log $K_{ow}$) to account for hydrophillic behaviour.

2. If log $K_{ow}$ is very large, i.e. greater than 6, estimated BCFs tend to be higher than measured BCFs. This is a particular problem when log $K_{ow}$ reaches 7 or 8. The reasons for this are not entirely clear. Gobas *et al.* (1987; 1988) address this issue in detail. A simple procedure is to assume that chemicals with a log $K_{ow}$ exceeding 6.5 have a ceiling value of 6.5. This first order correction improves the prediction of lab-measured BCFs, although the measured value itself may still be an underestimate of bioaccumulation potential.

3. Many compounds (e.g. polynuclear aromatic hydrocarbons) are metabolized and eliminated in some species at a rate which is a significant determinant of the tissue concentration. The higher the rate, the lower the measured BCF compared to an estimated value. It is very difficult, at present, to predict the extent of this decrease. If evidence suggests that metabolism (biotransformation) is operative, the person developing or using the BCFs should search for a reported "field" bioaccumulation factor. In some species, metabolism of a chemical causes a drastic increase in its toxicity. Therefore, metabolism does not always provide assurance of safety.

4. There may be a food chain effect. BCFs derived from laboratory data may underestimate, by a factor of about 10 to 15, the body burdens of hydrophobic (log $K_{ow}$ 5-7) chemicals in field-caught fish. This is an indication that consumption of contaminated food is the major route of exposure. Residue levels increase with fish size and age and a fish-water equilibrium may never be reached for compounds with a log $K_{ow}$ >5.

   If specific information on food chain effects is not available, a BAF for a top level predacious fish can be roughly estimated as the BCF multiplied by a factor of 3 for each trophic level below the fish. For example, if one views a food chain as an alga-zooplankton-minnow-predacious fish system and the BCF for the fish is 1000, then the BAF = 1000 x (3 + 3 + 3) = 9000.

5. Exposure time in a "steady-state" experiment was too short and a fish-water steady-state equilibrium was not reached such that the organism has a lower concentration than expected. For a series of related chemicals of increasing $K_{ow}$, elimination rate constants generally decrease (e.g. Bruggeman *et al.*,1981). In other words, the exposure time required to reach a steady-state concentration in biota ($t_{eq}$) increases with $K_{ow}$. The $t_{eq}$ also tends to increase with increasing size and lipid content of the exposed organism.

The following correlating equation, proposed by Gobas and Mackay (1987), can be used to judge the relevance of this phenomenon for a given data set:

$$1/k_2 = (V_L/Q_W) \times K_{ow} + (V_L/Q_L)$$

where V is the volume (litres) of lipid in the fish, Q is a transport parameter (litres per day), the subscripts L and W refer to lipid and water compartments within the fish and $k_2$ is the elimination (first order) rate constant.

$Q_W$ and $Q_L$ are organism-specific parameters, primarily dependent on fish body weight according to:

$$Q_W = 1.3 * M^{0.64}$$

$$Q_L = 0.014 * M^{0.6}$$

M = fish body weight between 0.1 and 1000 grams

It is thus possible to estimate: (1) $k_2$ (2) half-life time = $t_{1/2} = 0.693/k_2$ (3) time to steady-state equilibrium = $5 \times t_{1/2}$ for "every" chemical in "all" fish species if data are available for: (1) fish body weight (2) lipid content (3) chemical $K_{ow}$.

Growth dilution of tissue concentrations ($C_b$) may also be a significant determinant of the chemical concentration in biota during long term exposures. Estimates of biological half-lives based on body burden (i.e. $C_b \times M$) provide a sounder basis for half-life comparisons of the same chemical among studies and between species (Niimi, 1987).

6. There may be reduced bioavailability of the chemical in water. Sorption of the chemical to organic carbon-containing matter suspended in water may significantly reduce the concentration of truly dissolved, bioavailable chemical. If octanol is assumed to be an adequate surrogate for organic carbon, then the fraction of chemical which is in true solution is often approximated by:

   $$\text{fraction dissolved} = 1/(1 + K_{ow}\, C_o)$$

   where $C_o$ is the organic carbon content of water in g/g (not mg/l). If $\log K_{ow} = 4$ and $C_o = 10$ mg/l or $10^{-5}$ g/g, then the fraction dissolved is 0.91, 9% being sorbed and "unavailable".

   Experimental work to test the validity of this equation is lacking.

7. The chemical may display unusual or specific properties, for example, it may ionize (e.g. Saarikoski *et al.*, 1986), exhibit surface active (surfactant) properties, chelate, or vary in nature between metallic and organo-metallic forms. In such situations, case by case assessment is required.

While partitioning tendency of organic compounds and organo-metals can be related to a single parameter, octanol-water partition coefficient, no such simple generalization is possible for inorganic forms of metals. Mechanisms of uptake and storage of metals in aquatic biota are diverse and strongly influenced by factors such as chemical speciation and interactions with complexing ligands. Classical concepts of bioaccumulation typically do not hold for most metals.

8. If an organism is benthic in nature, tissue concentrations may be more indicative of those prevailing in the sediments than in the water column. In such situations, case by case assessment is required.

Standard test procedures or protocols do not always consider the potential problems described above. Therefore, best scientific judgement can and must be used to assess data on a case-by-case basis. Unless there are compelling arguments supporting an exception, the final BCF, standardized for fresh fish tissue having a lipid content (L) of 10%, can be determined as follows in order of preference:

(a) measured steady-state value from a laboratory test.

(b) projected steady-state value calculated from test data

(c) measured value from other types of laboratory tests

(d) measured bioaccumulation factor from a field study if the water concentration was relatively constant, "bioavailable" and less than known toxic levels.

(e) simulated value calculated as $BCF = L \times K_{ow}$ (described above).

(f) simulated value calculated using correlations with other physical-chemical properties (see Lyman *et al.*, 1982).

Caution must be exercised because erroneous conclusions may result from a comparison of BCFs expressed in different concentration units. Chemical concentration in whole fish or selected tissues are reported on the basis of wet weight, dry weight or lipid content (lipid normalized). While whole fish values can be used to assess aquatic environmental behaviour, muscle values may be more useful to evaluate consumable fish products for human health concerns. Reported water concentrations should reflect the truly dissolved (bioavailable) fraction of the chemical in water.

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## APPENDIX B – Mutagenicity: Acceptable Tests and Species

ACCEPTABLE TESTS

A. Assessment of Mutagenic Potential

The assessment of mutagenic or genotoxic potential may employ all available mutagenicity data, from tests with acceptable protocols, including data from aquatic as well as mammalian species. In addition, data from microbial or tissue culture test systems, with and without endogenous activation systems may be employed. Although such data are acceptable in this initial assessment, only data from tests employing aquatic organisms are acceptable in setting Objectives or Guidelines for mutagenicity.

B. Acceptable Tests for Objectives and Guidelines.

Only tests using fresh water organisms will be acceptable for setting mutagenicity Objectives. Data from tests using fresh water and marine organisms may be considered in setting Guidelines.
These lists of acceptable tests are examples and are not exclusive.

a. Mutagenicity Related Diseases

Data from these tests are considered when the substance in question is demonstrated to be mutagenic by other assays.

i Increased incidence of cancers or tumours in aquatic organisms. Waterborne exposure for significant proportion of life-cycle of aquatic species.

ii Increased incidence of mutagenicity related diseases in offspring of aquatic organisms including birth defects, heritable mutation or dominant lethal mutations.

b. Mutagenicity (resulting from exposure of whole organisms)

i Microbial assays such as the Ames test **without** endogenous activation.

ii Plant somatic mutation assays such as the *Tradescantia* staminal hair assay.

iii Somatic cell mutation (for example ouabain resistance) provided the exposure to the chemical was in-vivo (whole animal).

iv Host-mediated mutation assays.

v Anaphase or metaphase abnormalities of chromosomes.

vi Micronuclei.

c. Genotoxicity (resulting from exposure of whole organisms)

i DNA damage assays (Unscheduled DNA Synthesis)

ii Microbial DNA damage assays (Chromotest or Induct assays) in the absence of metabolic activation.

iii Sperm-head abnormality

iv Sister-chromatid exchanges

v DNA-adducts

ACCEPTABLE SPECIES

A. Vertebrate

Any fish species
Amphibians with life-stages resident in fresh water

B. Invertebrate

Freshwater invertebrates, either pelagic or benthic including annelids, crustaceans and molluscs. Data from tests using marine invertebrates, particularly those with freshwater relatives, would not be used in Objectives but may be considered in Guidelines.

C. Plant

Freshwater algae
Freshwater macrophytes, either wholly submergent, or those emergent from water with roots in the bottom substrate.

D. Bacteria

Bacteria shown to be resident in fresh water. Ames test *Salmonella* (without chemical activation) is an acceptable surrogate for freshwater bacteria.

# APPENDIX C – Worksheets and Tables

# TABLE 1: PHYSICAL-CHEMICAL PROPERTIES

| CHEMICAL: | CHEMICAL FORMULA: | CAS No: |
|---|---|---|
| | | |

## PROPERTIES

MOLECULAR WEIGHT (MW): _____

MELTING POINT: _____

BOILING POINT: _____

PHYSICAL STATE AT STANDARD TEMPERATURE AND PRESSURE: _____

pKa: _____

DENSITY (D): _____

MOLAR VOLUME (MW/D): _____

VAPOUR PRESSURE (Ps): _____

WATER SOLUBILITY (Cs): _____

HENRY'S LAW CONST.(Ps/Cs): _____

## PERSISTENCE

SURFACE WATER HALF LIFE: _____

AQUATIC FATE: _____

BREAKDOWN PRODUCTS: _____

## OCTANOL-WATER PARTITION COEFFICIENT ( Kow )

RANGE OF AVAILABLE Log Kow VALUES: _____

FINAL CHOSEN Log Kow VALUE: _____

## BASELINE UNCERTAINTY FACTOR FOR GUIDELINE DEVELOPMENT

IF Log Kow < 4.00, USE 1000 IF Log Kow ≥ 4.00, USE 10000

BASELINE UNCERTAINTY FACTOR: [ ]
(Enter this value into table 3)

# Table 2: Aquatic Toxicity Data Table

| CHEMICAL: | CAS No. | CONCENTRATION UNITS<br>mg/L |
|---|---|---|

| Test Conditions | | Species (life stage) | Toxicity End-point | pH | Temp (°C) | D.O. | Alk. | Hard. | Effect conc. | Data codes | Data Type | Ref. no. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ACUTE | VERTEBRATE | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | INVERT. | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| CHRONIC | VERTEBRATE | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | INVERT. | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | PLANT | | | | | | | | | | | |
| | | | | | | | | | | | | |

* - INDICATES VALUES ENTERED INTO TABLE 3

Assign 2 data codes, one from each of the following rows:

S = static R = static/renewal F = flowthrough

U = unmeasured nominal conc. M = measured conc.

PGI = Population Growth Impairment

(U.D.) = Unknown Duration

# TABLE 3: MUTAGENICITY DATA TABLE FOR -

| | SPECIES | END-POINT key (1) | TISSUE or ORGAN AFFECTED | LIFE STAGE and TIME or DURATION | TEST CONDITIONS | | CONC.'S TESTED (mg/L) | RESPONSE IN CONTROL and at CONC.'S TESTED | LOEL (mg/L) | DATA CODES key (2) | DATA QUALITY key (3) | REF. NO. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | ACTIV. | SOLVENT | | | | | | |
| VERTEBRATE | | | | | | | | | | | | |
| INVERTEBRATE | | | | | | | | | | | | |
| PLANT | | | | | | | | | | | | |
| MICROBIOLOGICAL | | | | | | | | | | | | |

key (1) END-POINT: AdD = DNA adducts; BsD = DNA strand breaks; CA = chromosomal aberrations; DLM = dominant lethal mutations; dmD = DNA damage/repair
HM = heritable mutations; HoM = host-mediated mutation; M = mutagenic in microbial systems; Mn = micronuclei; Neo = neoplasia;
SCE = sister chromatid exchange; Sha = spermhead abnormality; SM = somatic mutations; UDS = unscheduled DNA synthesis

key (2) DATA CODES: F = flowthrough; R = renewed static; S = static; M = measured toxicant concentrations; U = unmeasured toxicant concentrations

key (3) DATA QUALITY: P = primary(1°); S = secondary(2°); Aq = aquatic organism; NAq = non-aquatic organism

# Table 4: UNCERTAINTY FACTOR WORKSHEET

| CHEMICAL: | CAS No. | CONCENTRATION UNITS mg/L |
|---|---|---|
| | | |

| Test Conditions | | Species (life stage) | Toxicity End Point | Effect conc. | Data Codes | Data Type | Calibration Factor | No. and Reference |
|---|---|---|---|---|---|---|---|---|
| ACUTE | VERTEBRATE | | | | | | | |
| | | | | | | | | |
| | | | | | | | | |
| | INVERT. | | | | | | | |
| | | | | | | | | |
| CHRONIC | VERTEBRATE | | | | | | | |
| | | | | | | | | |
| | | | | | | | | |
| | INVERT. | | | | | | | |
| | | | | | | | | |
| | PLANT | | | | | | | |

## CALCULATION OF FINAL UNCERTAINTY FACTOR:

Since Log Kow ≥ 4.00, The Baseline Uncertainty Factor = 10000

Baseline Uncertainty Factor X Calibration Factors ( maximum number = 11 )

[ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ] X [ ]

= [ ] FINAL UNCERTAINTY FACTOR ( NOT TO BE LESS THAN A VALUE OF 13 )

CRITICAL VALUE + FINAL UNCERTAINTY FACTOR = PWQG OR INTERIM GUIDELINE VALUE

= _____ + _____ = _____mg/L

Assign 2 DATA CODES, one from each of the following rows:

S = static R = static/renewal F = flowthrough

U = unmeasured nominal conc. M = measured conc

DATA TYPE:

1° = Primary 2° = Secondary 3° = Simulated Data

? = Unknown (Default Data Quality = 2°)

## TABLE 4 (CONTINUED)

## CALCULATION OF THE FINAL UNCERTAINTY FACTOR

## CALIBRATION FACTORS FOR TOXICITY DATA

### ACUTE DATA

| | |
|---|---|
| PRIMARY ($1^{o}$) | 0.8 |
| SECONDARY ($2^{o}$) | 0.9 |
| SIMULATED BY QSAR ($3^{o}$) | 0.9 |

### CHRONIC DATA

| | |
|---|---|
| PRIMARY ($1^{o}$) | 0.5 |
| SECONDARY ($2^{o}$) | 0.7 |
| SIMULATED BY ACR ($3^{o}$) | 0.8 |
| PLANTS AND ALGAE | 0.9 |

## INSTRUCTIONS FOR COMPLETING THE UNCERTAINTY FACTOR WORKSHEET

1. A maximum of eleven (11) calibration factors may be used in calculating the final uncertainty factor.
2. For the purposes of setting Guidelines, all plant and algal data are considered secondary and chronic.
3. In the absence of a full set of measured acute and chronic toxicity data, simulated data from one ACR and/or one QSAR may be used.
4. The following data may be substituted to reduce the final uncertainty factor:

   -toxicity data on aquatic stages of amphibians may be used once as fish data.

   -aquatic toxicity data on protozoans may be used once as invertebrate data.
5. Guidelines cannot be based on plant, amphibian, protozoan and/or simulated data alone.
6. Unfilled acute data boxes may be filled with unused chronic data, provided other requirements (i.e. species diversity) are met. The acute calibration factor is used.

# Table 5: MUTAGENICITY GUIDELINE UNCERTAINTY FACTOR WORKSHEET

| CHEMICAL: | CAS No. | CONCENTRATION UNITS mg/L |
|---|---|---|
| | | |

| Test Conditions | | Species (life stage) | Toxicity End Point | LOEL (1) conc. | Calibration Factor (2) | No. and Reference |
|---|---|---|---|---|---|---|
| PRIMARY | VERTEBRATE | | | | | |
| | VERTEBRATE or INVERT. | | | | | |
| | PLANT or MICROBIAL | | | | | |
| SECONDARY | VERTEBRATE | | | | | |
| | INVERT. | | | | | |
| | PLANT | | | | | |
| | MICROBIAL | | | | | |

## CALCULATION OF FINAL UNCERTAINTY FACTOR:

Since Log Kow ≥ 4.00, The Baseline Uncertainty Factor = 10000

Baseline Uncertainty Factor X Calibration Factors ( maximum number = 9 )

[ ] x [ ] x [ ] x [ ] x [ ] x [ ] x [ ] x [ ] x [ ] x [ ]

= [ ] FINAL UNCERTAINTY FACTOR

CRITICAL VALUE ÷ FINAL UNCERTAINTY FACTOR = PWQG OR INTERIM GUIDELINE VALUE

= _____ ÷ _____ = _____ mg/L

(1) LOEL = Lowest concentration of chemical inducing an effect significantly above that of the control.
(2) Calbration Factor: Primary data = 0.4; Secondary data = 0.8

# Table 6: Data Requirements for Provincial Water Quality Objectives

## 1) Toxicity

All data must be primary, chronic ( or equivalent - use an asterisk to denote promotion of acute data to chronic data ), and marine or brackish species are not permitted.

### Fish

At Least:

| | |
|---|---|
| | one coldwater species |
| | one warmwater species |
| | one other warmwater or coldwater species |

With at Least:

| | |
|---|---|
| | one species resident in Ontario ( may be one of above ) |
| | one early lifestage endpoint |
| | one other whole organism chronic endpoint |

### Invertebrates

At Least:

| | |
|---|---|
| | one crustacean |
| | one non - crustacean |

With at Least:

| | |
|---|---|
| | no more than one tropical species |
| | one early lifestage endpoint |
| | one other chronic endpoint |

### Algae/Aquatic Plant

| | |
|---|---|
| | one algae or aquatic plant resident in temperate North America using scientific procedures and test conditions compatible with recognized algal bioassays |

# Table 6 (cont'd): Data Requirements for Provincial Water Quality Objectives

## 2) Bioaccumulation

One of:

| | |
|---|---|
| | fish consumption limit (e.g. Health and Welfare Canada Guidelines) |
| | an acceptable daily intake limit |
| | contaminant residue in aquatic biota value |

and:

| | |
|---|---|
| | A Bioconcentration Factor ≥ 1000 (In the absence of consumption limits, bioaccumulation may be significant and the Guideline setting process should be followed.) |

or:

| | |
|---|---|
| | A Bioconcentration Factor < 1000 (In the absence of consumption information, bioaccumulation is not considered to be significant.) |

If BCF data is unavailable:

| | |
|---|---|
| | Log Kow ≥ 4.00, then bioaccumulation is assumed to be significant and the Guideline setting process should be followed |

or:

| | |
|---|---|
| | Log Kow < 4.00, then bioaccumulation is assumed not to be significant |

# Table 6 (cont'd): Data Requirements for Provincial Water Quality Objectives

## 3) Mutagenicity

### a) For initial assessment:

| | |
|---|---|
| | Chemical is considered to be non-mutagenic (i.e. data from aminimum of two test systems, including tests for mutagenic as well as chromosomal damage endpoints, clearly demonstrating the chemical to be non-mutagenic) |
| | Chemical is considered to be mutagenic in aquatic or mammalian species |

### b) For setting PWQOs (a total of three studies are required for mutagenicity):

#### Vertebrates

All data must be primary and measured in whole aquatic organisms.
Marine and brackish tests are not permitted.

Data from at least one of the following three categories

| | |
|---|---|
| | fish - mutagenicity-related diseases |
| | fish - mutagenicity or chromosomal aberration |
| | other vertebrate mutagenicity or chromosomal aberration |

#### Invertebrates

Data from a maximum of two of the following three categories

| | |
|---|---|
| | invertebrate - mutagenicity or chromosomal aberration |
| | aquatic plant - mutagenicity or chromosomal aberration |
| | microbial - mutagenicity |

# FIG. C1: DERIVATION GRAPH -

| Toxicity Information Considered | | Species and Life Stage | Exposure and Duration | Concentration (mg/L) | Ref. No. |
|---|---|---|---|---|---|
| ACUTE | Vert. | | | | |
| | Invert. | | | | |
| | Plant | | | | |
| | other Organisms | | | | |
| CHRONIC | Vert. | | | | |
| | Invert. | | | | |
| | Plant | | | | |
| | other Organisms | | | | |
| MUTAGENICITY | Vert. | | | | |
| | Invert. | | | | |
| | Plant | | | | |
| | other Organisms | | | | |
| taste odour tainting | | | | | |
| BCF | | | | | |
| PWQG/PWQO Interim Guideline | | | | | |
| Other Criteria | | | | | |

o - Critical Value
✳-PWQG/Interim Guideline
■ - Toxicity endpoints
△ - Odour Protection Values
▲ - Taste Protection Values
□- Criteria of Other Agencies
● - Tainting Protection Values

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